



# STIC Search Report

## Biotech-Chem Library

STIC Database Tracking Number: 120882

TO: Edward Ward  
Location: 3d14/3d11  
Art Unit: 1654  
Friday, May 07, 2004  
Case Serial Number: 10/612885

3D11

From: Paul Schulwitz  
Location: Biotech-Chem Library  
REM-1A65  
Phone: (571)272-2527

[paul.schulwitz@uspto.gov](mailto:paul.schulwitz@uspto.gov)

### Search Notes

Examiner Ward,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

Paul Schulwitz  
Technical Information Specialist  
STIC Biotech/Chem Library  
(571)272-2527



05P 6/5

Access DB# 120882

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Edward Ward Examiner #: 67950 Date: May 2, 2004  
Art Unit: 1834 Phone Number: 471-277-0886 Serial Number: 11161273  
Mail Box and Bldg/Room Location: Room 3D11 / Room 3D14 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*  
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: \_\_\_\_\_

Inventors (please provide full names): Oleson, Lennart

Earliest Priority Filing Date: \_\_\_\_\_

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

1- AA-23 me Sequence #1 and the compound

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MAY - 3 2004  
STIC/STIC/STIC/STIC/STIC

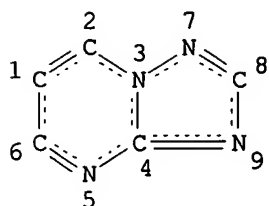
# Structures and seq id #1

Ward 10/612,885

May 7, 2004

=> d que 134

L13 STR



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DEFAULT ECLEVEL IS LIMITED

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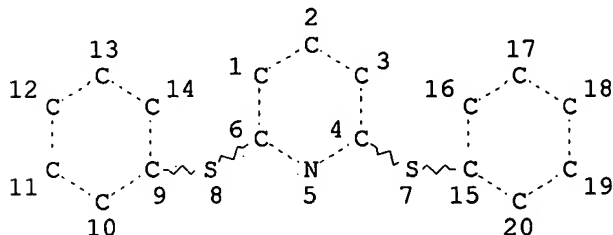
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L15 11751 SEA FILE=REGISTRY SSS FUL L13

L16 STR



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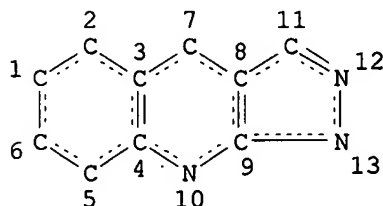
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L17 65 SEA FILE=REGISTRY SSS FUL L16

L18 STR



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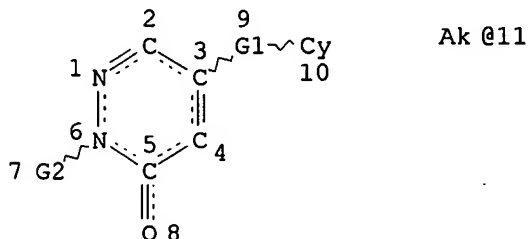
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L20 STR



VAR G1=O/S

VAR G2=H/11

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CONNECT IS E1 RC AT 11  
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## STEREO ATTRIBUTES: NONE

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~~L34~~ SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND (L15 OR L17 OR L19 OR L21)

=> d ibib abs l34

L34 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:41501 HCAPLUS

DOCUMENT NUMBER: 140:87744

TITLE: Affinity small molecules for the EPO receptor

INVENTOR(S): Olsson, Lennart; Naranda, Tatjana

PATENT ASSIGNEE(S): Receptron, Inc., USA

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

| PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------|------|----------|-----------------|----------|
| WO 2004005323 | A2   | 20040115 | WO 2003-US21394 | 20030703 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,  
UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,  
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,  
NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,  
GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-393360P P 20020703  
US 2002-393361P P 20020703  
US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

AB Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

L36 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 239133-03-0 REGISTRY

CN L-Tyrosine, L-glutamyl-L-arginyl-L-valyl-L- $\alpha$ -glutamyl-L-isoleucyl-L-leucyl-L- $\alpha$ -glutamylglycyl-L-arginyl-L-threonyl-L- $\alpha$ -glutamyl-L-cysteinyl-L-valyl-L-leucyl-L-seryl-L-asparaginyl-L-leucyl-L-arginylglycyl-L-arginyl-L-threonyl-L-arginyl- (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN 11: PN: US6333031 SEQID: 11 claimed protein

CN 1: PN: WO2004005323 SEQID: 1 unclaimed sequence

CN 30: PN: WO03020746 SEQID: 30 unclaimed sequence

CN 30: PN: WO2004020588 SEQID: 30 unclaimed sequence

FS PROTEIN SEQUENCE; STEREOSEARCH

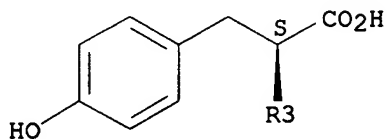
MF C115 H198 N40 O36 S

SR CA

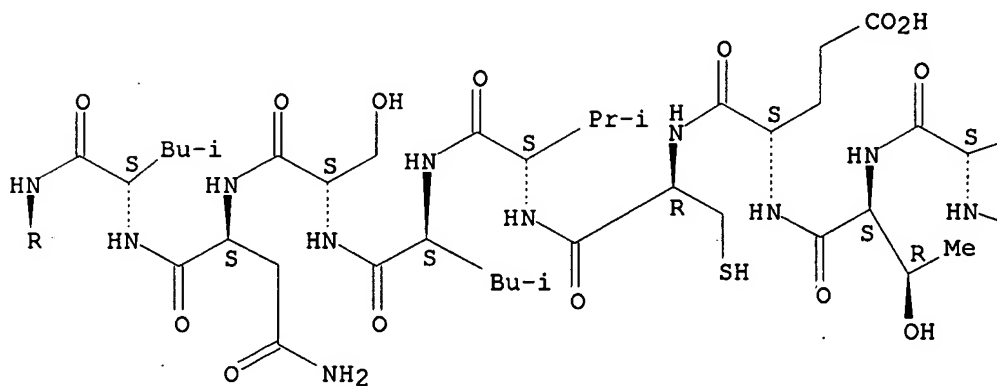
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

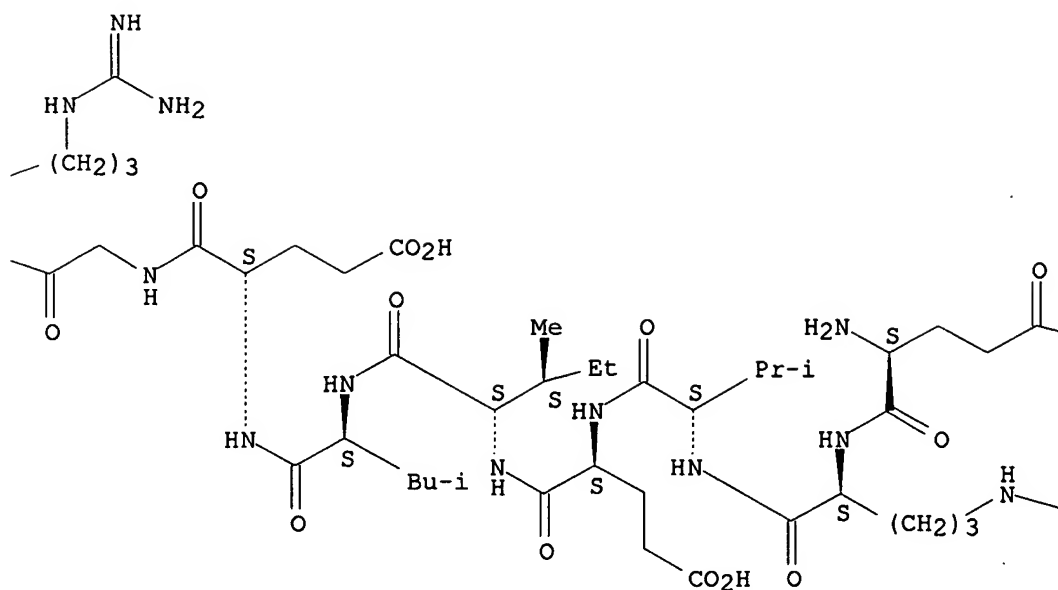
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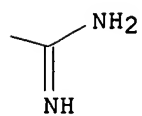
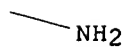
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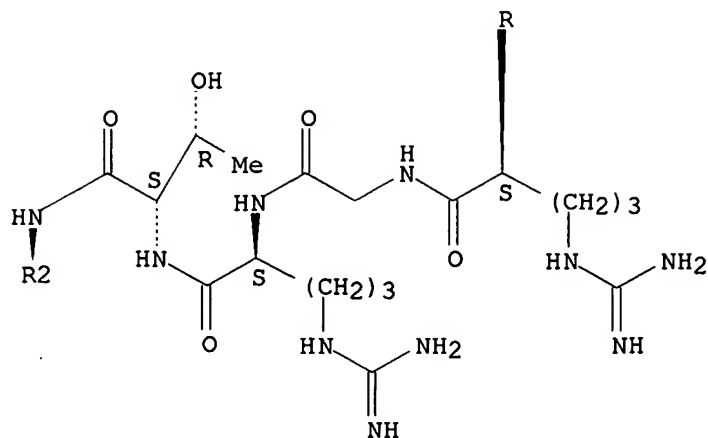
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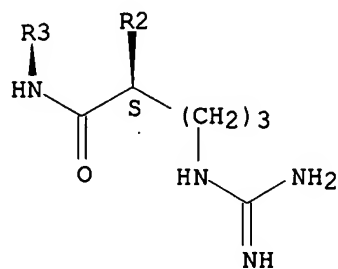
PAGE 2-C



PAGE 3-A



PAGE 4-A



7 REFERENCES IN FILE CA (1907 TO DATE)  
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

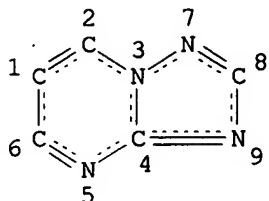
# Structures + Text

Ward 10/612,885

May 7, 2004

=> d que

L10 1 SEA FILE=REGISTRY ABB=ON PLU=ON 11096-26-7  
 L11 1095 SEA FILE=HCAPLUS ABB=ON PLU=ON ERYTHROPOIETIN RECEPTORS+OLD/C  
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 L13 STR

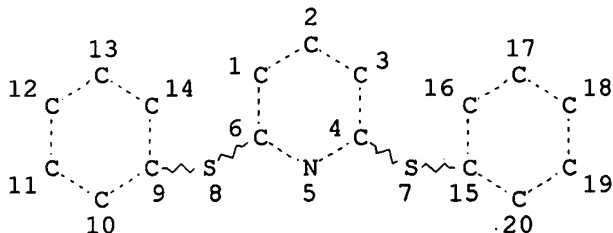


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 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE  
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 L16 STR

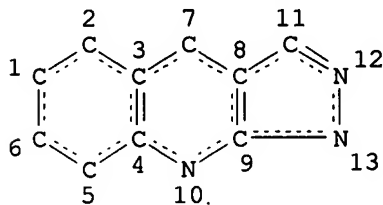


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NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE  
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 L18 STR



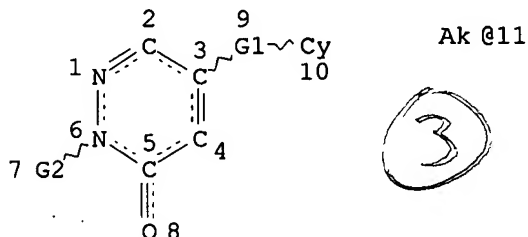
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE  
L19 1779 SEA FILE=REGISTRY SSS FUL L18  
L20 STR



VAR G1=O/S  
VAR G2=H/11  
NODE ATTRIBUTES:  
CONNECT IS E1 RC AT 11  
DEFAULT MLEVEL IS ATOM  
GGCAT IS UNS AT 10  
GGCAT IS LOC AT 11  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE  
L21 158 SEA FILE=REGISTRY SSS FUL L20  
L22 2621 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 OR L17 OR L19 OR L21  
~~L24 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (L11 OR L10 OR EPO OR~~  
ERYTHROPO?) AND L22

~~=> [L24] [HCAPLUS] [HITTING] [HITTING]~~

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2004:41501 HCAPLUS  
DOCUMENT NUMBER: 140:87744  
TITLE: Affinity small molecules for the EPO receptor  
INVENTOR(S): Olsson, Lennart; Naranda, Tatjana  
PATENT ASSIGNEE(S): Receptron, Inc., USA  
SOURCE: PCT Int. Appl., 85 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.   | KIND   | DATE     | APPLICATION NO. | DATE       |
|--|--|----------|-----------------|------------|
| WO 2004005323  | A2   | 20040115 | WO 2003-US21394 | 20030703   |
| <p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p> |  |          |                 |            |
| PRIORITY APPLN. INFO.:   |  |          | US 2002-393360P | P 20020703 |
|  |  |          | US 2002-393361P | P 20020703 |
|  |  |          | US 2002-394110P | P 20020703 |
| OTHER SOURCE(S): MARPAT 140:87744  |  |          |                 |            |
| AB   | Compds. are provided that complex with the modulating domain of <b>erythropoietin</b> receptor ( <b>EPO-R</b> ) for use with <b>EPO</b> -R to determine the presence of <b>EPO-R</b> , the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by <b>EPO-R</b> into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine. |          |                 |            |
| IC   | ICM C07K   |          |                 |            |
| CC   | 1-12 (Pharmacology)  |          |                 |            |
|  | Section cross-reference(s): 2  |          |                 |            |
| ST   | <b>EPO</b> receptor modulator small mol  |          |                 |            |
| IT   | Proteins   |          |                 |            |
|  | RL: BSU (Biological study, unclassified); BIOL (Biological study) (Bcl-xL, expression; affinity small mols. for <b>erythropoietin</b> ( <b>EPO</b> ) receptor and <b>EPO</b> receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)   |          |                 |            |
| IT   | Peptides, biological studies   |          |                 |            |
|  | RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) ( <b>EPO</b> receptor modulating sequence; affinity small mols. for <b>erythropoietin</b> ( <b>EPO</b> ) receptor and <b>EPO</b> receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)   |          |                 |            |
| IT   | Cell membrane  |          |                 |            |
|  | (EPO receptors of; affinity small mols. for <b>erythropoietin</b> ( <b>EPO</b> ) receptor and <b>EPO</b> receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)   |          |                 |            |
| IT   | Anemia (disease)   |          |                 |            |
|  | Cell proliferation   |          |                 |            |
|  | Combinatorial library  |          |                 |            |
|  | Drug delivery systems  |          |                 |            |
|  | Drug screening   |          |                 |            |
|  | Erythrocyte  |          |                 |            |

**Erythropoiesis**

Hematocrit

Hematopoietic precursor cell

Human

Reticulocyte

(affinity small mols. for **erythropoietin (EPO)**  
receptor and **EPO** receptor modulating sequence in relation to  
modulating the response to the stimulus of hematopoietic or neuronal  
cells and treatment of anemia)

IT **Erythropoietin receptors**

RL: BSU (Biological study, unclassified); BUU (Biological use,  
unclassified); BIOL (Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)**  
receptor and **EPO** receptor modulating sequence in relation to  
modulating the response to the stimulus of hematopoietic or neuronal  
cells and treatment of anemia)

## IT Nerve

(neuron; affinity small mols. for **erythropoietin (EPO)**  
) receptor and **EPO** receptor modulating sequence in relation  
to modulating the response to the stimulus of hematopoietic or neuronal  
cells and treatment of anemia)

## IT Cytoprotective agents

(neuroprotective; affinity small mols. for **erythropoietin (EPO)**  
**EPO** receptor and **EPO** receptor modulating sequence in  
relation to modulating the response to the stimulus of hematopoietic or  
neuronal cells and treatment of anemia)

## IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

56347-20-7 63901-48-4 90559-98-1

90815-61-5 113967-71-8 113967-74-1

194342-06-8 212074-47-0 244167-89-3

245082-87-5 245413-82-5 259683-29-9

261704-08-9 261704-09-0 262291-81-6

263267-38-5 287728-46-5 303145-64-4

303145-73-5 338793-16-1 645337-19-5

645337-20-8 645337-21-9 645337-22-0

645337-23-1 645337-24-2 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use,  
unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)**  
receptor and **EPO** receptor modulating sequence in relation to  
modulating the response to the stimulus of hematopoietic or neuronal  
cells and treatment of anemia)

IT 11096-26-7, **Erythropoietin**

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)**  
receptor and **EPO** receptor modulating sequence in relation to  
modulating the response to the stimulus of hematopoietic or neuronal  
cells and treatment of anemia)

## IT 239133-03-0 645415-22-1

RL: PRP (Properties)

(unclaimed sequence; affinity small mols. for the **EPO**  
receptor)

## IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

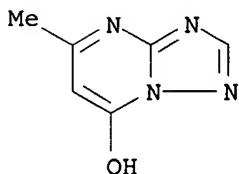
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 245082-87-5 245413-82-5 259683-29-9  
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 263267-38-5 287728-46-5 303145-64-4  
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RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)** receptor and **EPO** receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

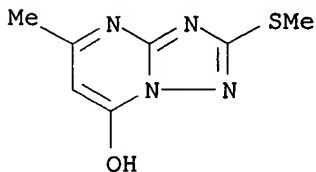
RN 2503-56-2 HCAPLUS

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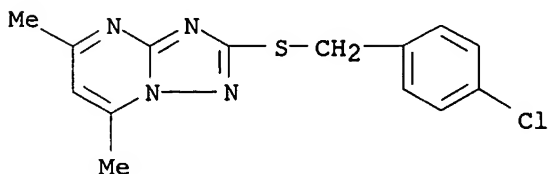
RN 40775-78-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl-2-(methylthio)- (9CI) (CA INDEX NAME)



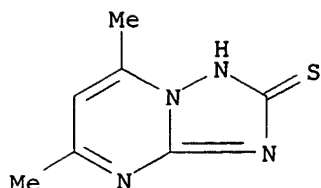
RN 51646-16-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[ (4-chlorophenyl)methyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)



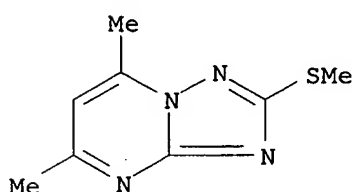
RN 51646-17-4 HCAPLUS

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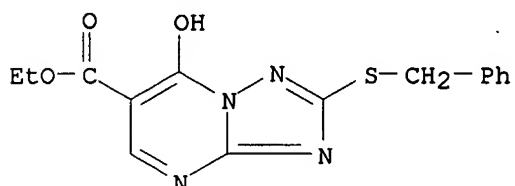
RN 51646-19-6 HCAPLUS

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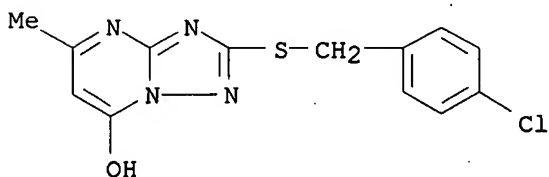
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CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-hydroxy-2-[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



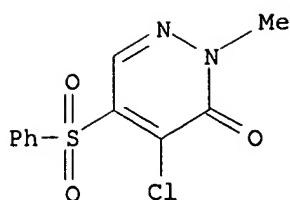
RN 56347-20-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[[4-(4-chlorophenyl)methyl]thio]-5-methyl- (9CI) (CA INDEX NAME)



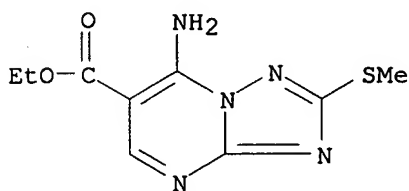
RN 63901-48-4 HCAPLUS

CN 3(2H)-Pyridazinone, 4-chloro-2-methyl-5-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



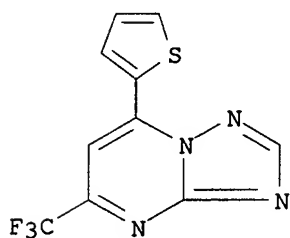
RN 90559-98-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)-, ethyl ester (9CI) (CA INDEX NAME)



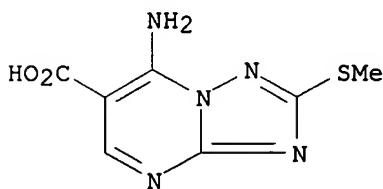
RN 90815-61-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(2-thienyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



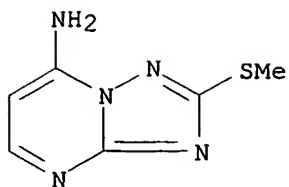
RN 113967-71-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)- (9CI) (CA INDEX NAME)



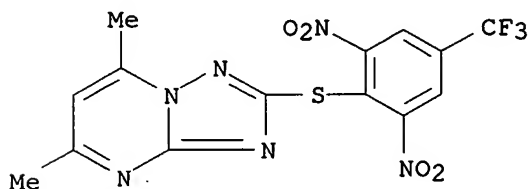
RN 113967-74-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 2-(methylthio)- (9CI) (CA INDEX NAME)



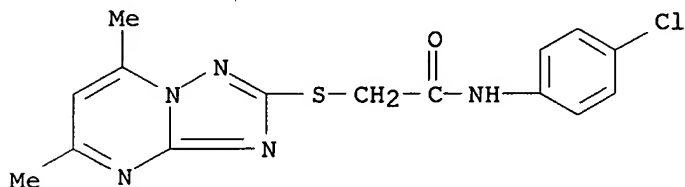
RN 194342-06-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[2,6-dinitro-4-(trifluoromethyl)phenyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)



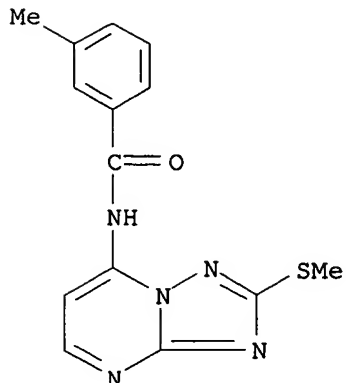
RN 212074-47-0 HCAPLUS

CN Acetamide, N-(4-chlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)

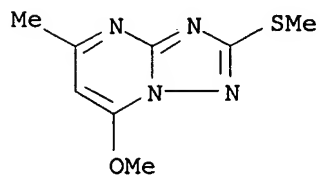


RN 244167-89-3 HCAPLUS

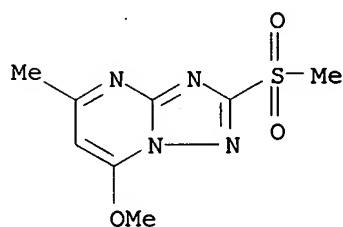
CN Benzamide, 3-methyl-N-[2-(methylthio)[1,2,4]triazolo[1,5-a]pyrimidin-7-yl]- (9CI) (CA INDEX NAME)



RN 245082-87-5 HCAPLUS

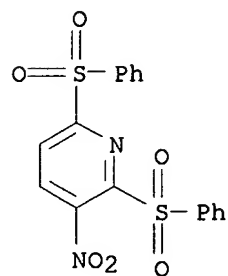
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylthio)- (9CI)  
(CA INDEX NAME)

RN 245413-82-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylsulfonyl)-  
(9CI) (CA INDEX NAME)

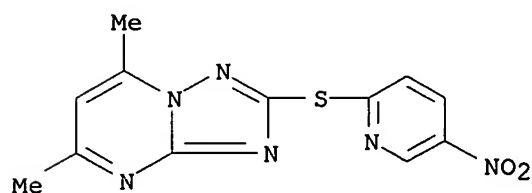
RN 259683-29-9 HCAPLUS

CN Pyridine, 3-nitro-2,6-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



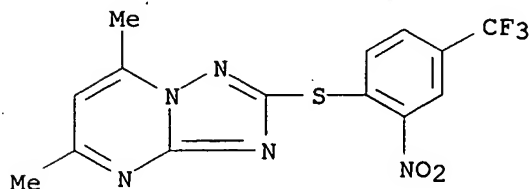
RN 261704-08-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(5-nitro-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)



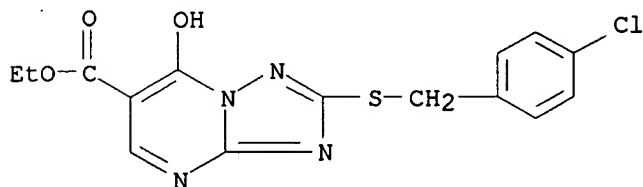
RN 261704-09-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[[2-nitro-4-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



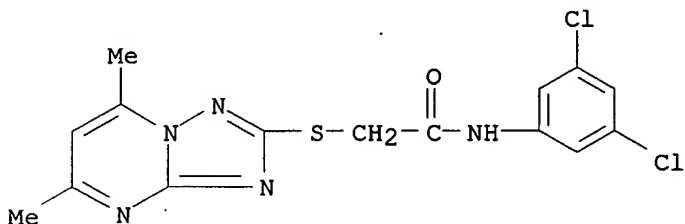
RN 262291-81-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 2-[[[4-chlorophenyl)methyl]thio]-7-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



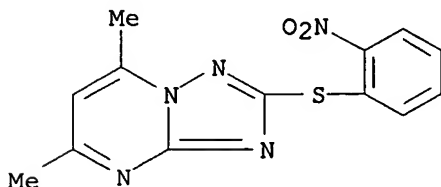
RN 263267-38-5 HCAPLUS

CN Acetamide, N-(3,5-dichlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)

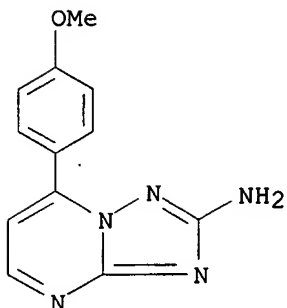


RN 287728-46-5 HCAPLUS

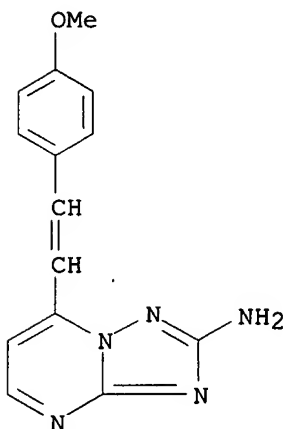
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



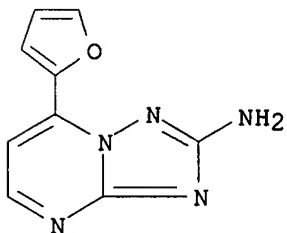
RN 303145-64-4 HCAPLUS  
CN [1,2,4]Triazolo[1,5-a]pyrimidin-2-amine, 7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 303145-73-5 HCAPLUS  
CN [1,2,4]Triazolo[1,5-a]pyrimidin-2-amine, 7-[2-(4-methoxyphenyl)ethenyl]- (9CI) (CA INDEX NAME)

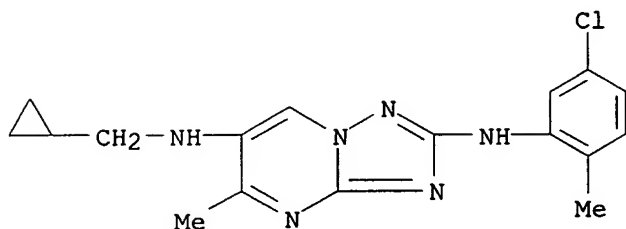


RN 338793-16-1 HCAPLUS  
CN [1,2,4]Triazolo[1,5-a]pyrimidin-2-amine, 7-(2-furanyl)- (9CI) (CA INDEX NAME)



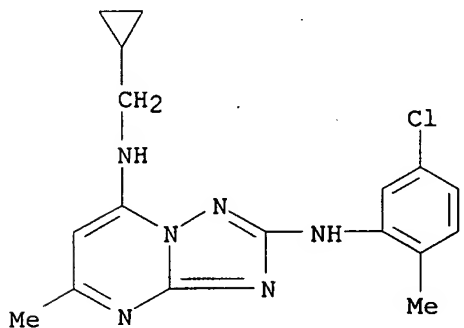
RN 645337-19-5 HCAPLUS  
CN [1,2,4]Triazolo[1,5-a]pyrimidine-2,6-diamine, N2-(5-chloro-2-methylphenyl)-

N6-(cyclopropylmethyl)-5-methyl- (9CI) (CA INDEX NAME)



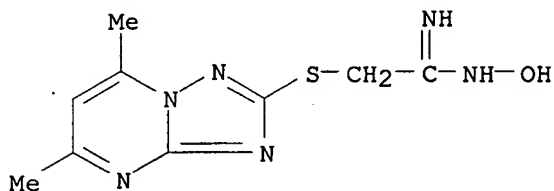
RN 645337-20-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-2,7-diamine, N2-(5-chloro-2-methylphenyl)-  
N7-(cyclopropylmethyl)-5-methyl- (9CI) (CA INDEX NAME)



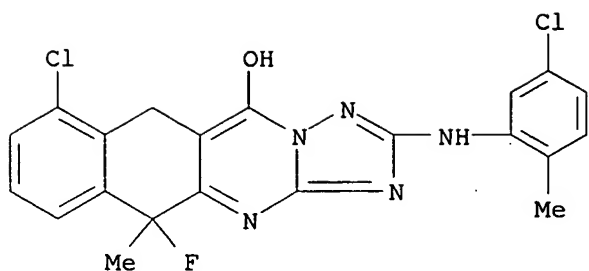
RN 645337-21-9 HCAPLUS

CN Ethanimidamide, 2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]-  
N-hydroxy- (9CI) (CA INDEX NAME)



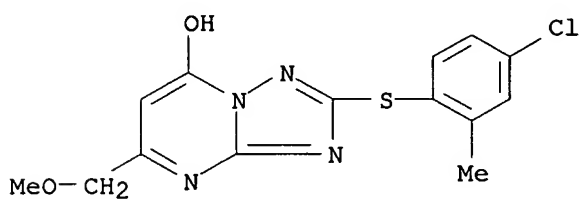
RN 645337-22-0 HCAPLUS

CN Benzo[g][1,2,4]triazolo[5,1-b]quinazolin-11-ol, 9-chloro-2-[(5-chloro-2-methylphenyl)amino]-5-fluoro-5,10-dihydro-5-methyl- (9CI) (CA INDEX NAME)



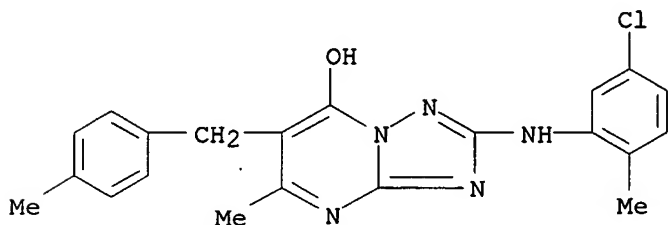
RN 645337-23-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[(4-chloro-2-methylphenyl)thio]-5-(methoxymethyl)- (9CI) (CA INDEX NAME)



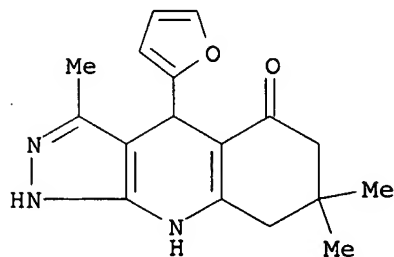
RN 645337-24-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[(5-chloro-2-methylphenyl)amino]-5-methyl-6-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 645337-25-3 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-(2-furanyl)-1,4,6,7,8,9-hexahydro-3,7,7-trimethyl- (9CI) (CA INDEX NAME)



IT 11096-26-7, Erythropoietin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(affinity small mols. for **erythropoietin (EPO)**  
receptor and **EPO** receptor modulating sequence in relation to  
modulating the response to the stimulus of hematopoietic or neuronal  
cells and treatment of anemia)

RN 11096-26-7 HCAPLUS

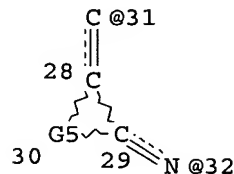
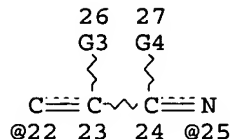
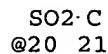
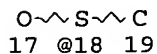
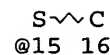
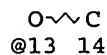
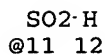
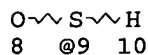
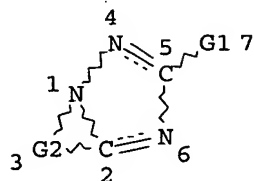
CN Erythropoietin (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

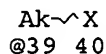
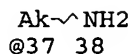
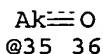
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L9

STR



Ak @34



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VAR G2=22-1 25-2/31-1 32-2

VAR G3=H/33

VAR G4=H/34/35/37/39

REP G5=(1-20) A

NODE ATTRIBUTES:

NSPEC IS RC AT 14

NSPEC IS RC AT 16

NSPEC IS RC AT 19

NSPEC IS RC AT 21

NSPEC IS RC AT 33

CONNECT IS E1 RC AT 8

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CONNECT IS E2 RC AT 15

CONNECT IS E1 RC AT 17

CONNECT IS E3 RC AT 18

CONNECT IS E1 RC AT 34

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GGCAT IS LOC AT 37

GGCAT IS LOC AT 39

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

L11 3288 SEA FILE=REGISTRY SSS FUL L9

L18 678 SEA FILE=HCAPLUS ABB=ON PLU=ON L11(L)BIOL/RL

L19 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L11(L)MODULAT?

L20 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L19

L23 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND (NEURON? OR HEMATOPOI?  
OR ANEMI?)  
L24 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 OR L20

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L24 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:80683 HCAPLUS

DOCUMENT NUMBER: 140:128433

TITLE: Preparation of piperazinyl-2(1H)-pyrazinones for  
treatment of 5-HT2A receptor-related disorders

INVENTOR(S): Nilsson, Bjoern; Thor, Markus; Cernerud, Magnus;  
Lundstroem, Helena

PATENT ASSIGNEE(S): Biovitrum Ab, Swed.

SOURCE: PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

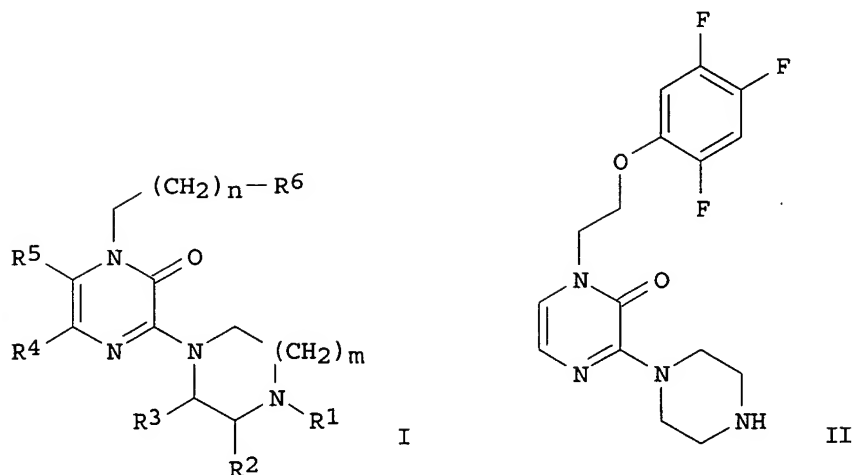
PATENT INFORMATION:

| PATENT NO.    | KIND   | DATE     | APPLICATION NO. | DATE     |
|---------------|--|----------|-----------------|----------|
| WO 2004009586 | A1   | 20040129 | WO 2003-SE1102  | 20030625 |
| W:            | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |          |
| RW:           | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG   |          |                 |          |

PRIORITY APPLN. INFO.: SE 2002-2287 A 20020719  
US 2002-426240P P 20021114

OTHER SOURCE(S): MARPAT 140:128433

GI



AB Title compds. I [wherein m = 1-2; n = 0-4; R1 = H, (methoxy)alkyl, 2-hydroxyethyl, alkoxycarbonyl, or (un)substituted (hetero)arylalkyl or (hetero)aryloxyalkyl; R2 and R3 = independently H or Me; R4 and R5 = independently H, halo, or Me; or R4 and R5 together with the ring to which the C atoms are attached = a 1H-quinoxalin-2-one nucleus; R6 = (un)substituted (hetero)aryloxy, (hetero)arylthio, (hetero)arylamino, (hetero)aryl, or (hetero)arylcarbonyl; with provisos; and pharmaceutically acceptable salts, hydrates, geometrical isomers, tautomers, optical isomers, N-oxides, or prodrugs thereof] were prepared as 5-HT<sub>2A</sub> receptor modulators. For example, condensation of 2,4,5-trifluorophenol with 2-[3-(4-tert-butoxycarbonyl-1-piperazinyl)pyrazinyl]ethanol in the presence of TMAD and polymer-bound PPh<sub>3</sub> in CH<sub>2</sub>Cl<sub>2</sub>, followed by deprotection with TFA/CH<sub>2</sub>Cl<sub>2</sub>/H<sub>2</sub>O and salt formation gave II•HCl (85%). The latter displaced 3H-labeled LSD bound to membranes, prepared from transfected CHO cell line stably expressing the human 5-HT<sub>2A</sub> receptor protein, with a receptor affinity value of K<sub>i</sub> = 2.2 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of 5-HT<sub>2A</sub> receptor-related disorders, such as Raynaud's phenomenon, hypertension, fibromyalgia, thrombotic disorders, Alzheimer's disease, depression, COPD, glaucoma, eating disorders, etc. (no data).

IC. ICM C07D239-02

ICS C07D295-033; A61K031-496; A61P003-04; A61P003-10; A61P009-00; A61P015-00; A61P025-28; A61P025-24

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

IT 651046-48-9P 651046-50-3P, 1-[2-[(2-Oxo-2H-chromen-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651046-52-5P, 3-(1-Piperazinyl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651046-53-6P, 3-(1-Piperazinyl)-1-[2-(2,3,5,6-tetrafluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651046-54-7P, 1-[2-(2,3,4,5,6-Pentafluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651046-55-8P, 1-[2-(4-Chloro-2-fluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-56-9P, 1-[2-(3-Cyanophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-57-0P, 1-[2-(4-Cyclopentylphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-58-1P, 1-[2-[(1,2-Benzisoxazol-3-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one dihydrochloride 651046-59-2P, 1-[2-(3-Methoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-60-5P, 1-[2-[3-(Butyloxy)phenoxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one

651046-61-6P, 1-[2-[(1,1'-Biphenyl)-3-yl]oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-62-7P, 3-(1-Piperazinyl)-1-[2-(2,3,4-trifluorophenoxy)ethyl]-1H-pyrazin-2-one  
 651046-63-8P, 1-[2-(2,3-Dichlorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-64-9P, 1-[2-[(1,3-Benzodioxol-5-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-65-0P, 1-[2-(2,4-Difluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
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 651046-67-2P, 1-[2-[(2-Oxo-1,3-benzoxathiol-5-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-68-3P, 1-[2-(3-Hydroxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
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 hydrochloride 651046-72-9P, 1-[2-[3-(N,N-Dimethylamino)phenoxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 fumarate 651046-76-3P, 3-(1-Piperazinyl)-1-[2-[3-(trifluoromethyl)phenoxy]ethyl]-1H-pyrazin-2-one  
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 trifluoroacetate 651046-85-4P, 1-[2-(2,6-Difluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-86-5P, 1-[2-(2,6-Difluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-87-6P, 1-[2-(2-Cyanophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-88-7P, 1-[2-(2-Cyanophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-89-8P, 1-[2-(4-Trifluoromethylphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-90-1P, 1-[2-(4-Trifluoromethylphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-91-2P, 1-[2-(4-Bromophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-92-3P, 1-[2-(4-Bromophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-93-4P, 1-[2-(4-Phenoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-94-5P, 1-[2-(4-Phenoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-95-6P, 1-[2-(4-Fluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-96-7P, 1-[2-(4-Fluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-97-8P, 1-[2-(4-Isopropylphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651046-98-9P, 1-[2-(4-Isopropylphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651046-99-0P, 1-[2-(2,4,5-Trichlorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651047-00-6P, 1-[2-(2,4,5-Trichlorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651047-01-7P, 1-[2-(2-Methylthiophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651047-02-8P, 1-[2-(2-Methylthiophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651047-03-9P, 1-[2-(3-Methoxyphenylthio)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651047-04-0P, 1-[2-(3-Methoxyphenylthio)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651047-05-1P, 1-[2-(4-Allyl-2-methoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651047-06-2P, 1-[2-(4-Allyl-2-methoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651047-07-3P, 1-[2-[(5,6,7,8-Tetrahydronaphthalen-2-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 651047-08-4P, 1-[2-[(5,6,7,8-Tetrahydronaphthalen-2-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one  
 trifluoroacetate 651047-09-5P, 1-[2-(2,6-Difluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one  
 651047-10-8P,

1-[2-(2,6-Difluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-11-9P, 1-[2-(4-Trifluoromethylphenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-12-0P, 1-[2-(4-Trifluoromethylphenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-13-1P, 1-[2-(4-Bromophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-14-2P, 1-[2-(4-Bromophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-15-3P, 1-[2-(Phenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-16-4P, 1-[2-(Phenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-17-5P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-18-6P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-19-7P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-20-0P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-21-1P, 1-[2-(4-Fluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-22-2P, 1-[2-(4-Fluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-23-3P, 1-[2-(4-Isopropylphenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-24-4P, 1-[2-(4-Isopropylphenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-25-5P, 1-[2-(2-Methylthiophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-26-6P, 1-[2-[2-(Methylthio)phenoxy]ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-27-7P, 1-(2,4,5-Trifluorobenzyl)-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-28-8P, 1-(2,4,5-Trifluorobenzyl)-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-31-3P, 1-[3-(2,4,5-Trifluorophenyl)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-32-4P, 1-[3-(2,4,5-Trifluorophenyl)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-36-8P, 1-[(2,3-Dihydrobenzo[1,4]dioxin-2-yl)methyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-37-9P, 1-[(2,3-Dihydrobenzo[1,4]dioxin-2-yl)methyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-39-1P, 3-(Piperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-quinoxalin-2-one 651047-40-4P, 3-(Piperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-quinoxalin-2-one trifluoroacetate 651047-45-9P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(4-n-butyl-1-piperazinyl)-1H-pyrazin-2-one 651047-47-1P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-[4-(2-methoxyethyl)-1-piperazinyl]-1H-pyrazin-2-one 651047-48-2P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-[4-(2-methoxyethyl)-1-piperazinyl]-1H-pyrazin-2-one trifluoroacetate 651047-49-3P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(4-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-52-8P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(4-isopropyl-1-piperazinyl)-1H-pyrazin-2-one 651047-55-1P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651047-57-3P, 1-[2-(4-Cyanophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one maleate 651047-59-5P, 1-[4-(2,4,5-Trifluorophenoxy)butyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-60-8P, 1-[4-(2,4,5-Trifluorophenoxy)butyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-64-2P, 1-[3-(2,4,5-Trifluorophenoxy)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-65-3P, 1-[3-(2,4,5-Trifluorophenoxy)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-69-7P, 3-[4-(1-Phenylethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651047-70-0P, 3-[4-(2-Phenoxyethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651047-71-1P, 3-[4-(2-Phenylethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651047-72-2P, 3-(4-Benzylpiperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-

2-one hydrochloride 651047-73-3P, 3-((2R)-2-Methylpiperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one 651047-74-4P, 3-((2R)-2-Methylpiperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one trifluoroacetate 651047-76-6P, 1-[2-(4-Allyl-2-methoxyphenoxy)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one maleate 651047-78-8P, 3-(Piperazin-1-yl)-1-[2-(3-thienyl)ethyl]-1H-pyrazin-2-one 651047-79-9P, 3-(Piperazin-1-yl)-1-[2-(3-thienyl)ethyl]-1H-pyrazin-2-one maleate 651047-80-2P, 3-(Piperazin-1-yl)-1-[2-(2-thienyl)ethyl]-1H-pyrazin-2-one 651047-81-3P, 3-(Piperazin-1-yl)-1-[2-(2-thienyl)ethyl]-1H-pyrazin-2-one trifluoroacetate 651047-82-4P, 1-[2-(1H-Indol-3-yl)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-83-5P, 1-[2-(1H-Indol-3-yl)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-84-6P, 1-[2-[(2,3-Dihydro-1,4-benzodioxin-5-yl)oxy]ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-85-7P, 1-[2-[(2,3-Dihydro-1,4-benzodioxin-5-yl)oxy]ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-87-9P, 1-[2-(Phenylthio)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-88-0P, 1-[2-(Phenylthio)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-89-1P, 1-(3-Oxo-3-phenylpropyl)-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-90-4P, 1-(3-Oxo-3-phenylpropyl)-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-91-5P, 1-[3-(4-Fluorophenyl)-3-oxopropyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-92-6P, 1-[3-(4-Fluorophenyl)-3-oxopropyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-96-0P, 1-[2-(2-Fluoro-4-nitrophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-97-1P, 1-[2-[(2-Oxo-2H-chromen-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-98-2P, 3-(1-Piperazinyl)-1-[2-(2,3,5,6-tetrafluorophenoxy)ethyl]-1H-pyrazin-2-one 651047-99-3P, 1-[2-(2,3,4,5,6-Pentafluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651048-00-9P, 1-[2-[(Benzisoxazol-3-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651048-01-0P, 3-(1-Piperazinyl)-1-[2-[(6-quinoxalinyloxy)ethyl]-1H-pyrazin-2-one 651048-03-2P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651048-04-3P, 3-[4-(1-Phenylethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one 651048-05-4P, 3-[4-(2-Phenoxyethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);

USES (Uses)

(5-HT2A receptor modulator; preparation of piperazinylpyrazinones for treatment of 5-HT2A receptor-related disorders)

IT 651047-55-1P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651048-03-2P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one

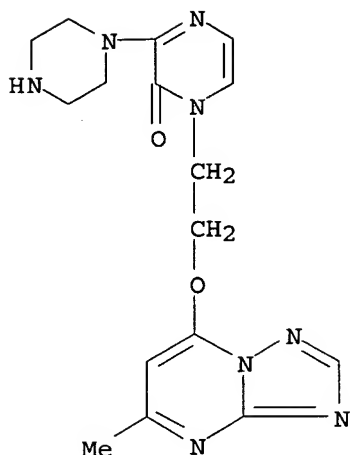
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);

USES (Uses)

(5-HT2A receptor modulator; preparation of piperazinylpyrazinones for treatment of 5-HT2A receptor-related disorders)

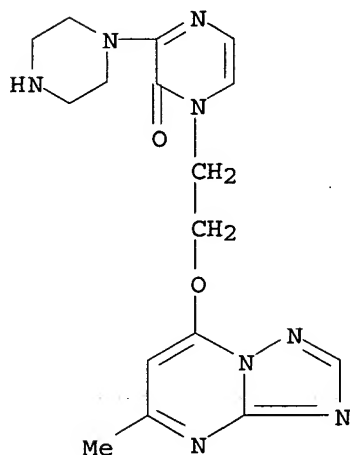
RN 651047-55-1 HCAPLUS

CN 2(1H)-Pyrazinone, 1-[2-[(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 651048-03-2 HCAPLUS  
 CN 2(1H)-Pyrazinone, 1-[2-[(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2004:41501 HCAPLUS  
 DOCUMENT NUMBER: 140:87744  
 TITLE: Affinity small molecules for the EPO receptor  
 INVENTOR(S): Olsson, Lennart; Naranda, Tatjana  
 PATENT ASSIGNEE(S): Receptron, Inc., USA  
 SOURCE: PCT Int. Appl., 85 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| WO 2004005323   | A2   | 20040115 | WO 2003-US21394 | 20030703 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,<br>CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,<br>GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,<br>LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,<br>PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,<br>UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM<br>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,<br>CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,<br>NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,<br>GW, ML, MR, NE, SN, TD, TG |      |          |                 |          |

PRIORITY APPLN. INFO.:  
 US 2002-393360P P 20020703  
 US 2002-393361P P 20020703  
 US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

AB Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

IC ICM C07K

CC 1-12 (Pharmacology)

Section cross-reference(s): 2

IT Proteins

RL: BSU (Biological study, unclassified); BIOL (Biological study) (Bcl-xL, expression; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Peptides, biological studies

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (EPO receptor modulating sequence; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Cell membrane

(EPO receptors of; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT **Anemia** (disease)

Cell proliferation

Combinatorial library

Drug delivery systems

Drug screening

Erythrocyte

Erythropoiesis

Hematocrit

**Hematopoietic** precursor cell

Human

Reticulocyte

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Erythropoietin receptors

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Nerve

(**neuron**; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Cytoprotective agents

(neuroprotective; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

56347-20-7 63901-48-4 90559-98-1 90815-61-5

113967-71-8 113967-74-1 194342-06-8

212074-47-0 244167-89-3 245082-87-5

245413-82-5 259683-29-9 261704-08-9

261704-09-0 262291-81-6 263267-38-5

287728-46-5 303145-64-4 303145-73-5 338793-16-1

645337-19-5 645337-20-8 645337-21-9 645337-22-0

645337-23-1 645337-24-2 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor **modulating** sequence in relation to **modulating** the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT 11096-26-7, Erythropoietin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

56347-20-7 90559-98-1 90815-61-5

113967-71-8 113967-74-1 194342-06-8

212074-47-0 244167-89-3 245082-87-5

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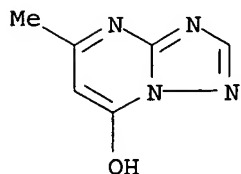
645337-21-9

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

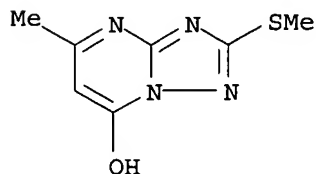
RN 2503-56-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl- (9CI) (CA INDEX NAME)



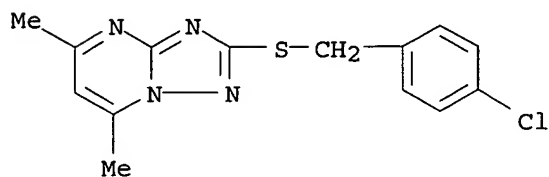
RN 40775-78-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl-2-(methylthio)- (9CI) (CA INDEX NAME)



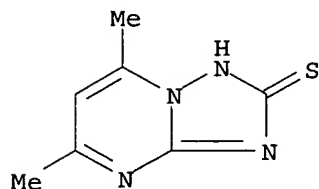
RN 51646-16-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[4-chlorophenyl)methyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)



RN 51646-17-4 HCAPLUS

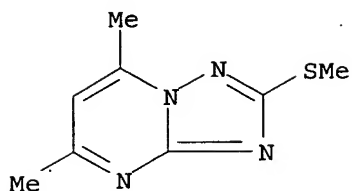
CN [1,2,4]Triazolo[1,5-a]pyrimidine-2(1H)-thione, 5,7-dimethyl- (9CI) (CA INDEX NAME)



RN 51646-19-6 HCAPLUS

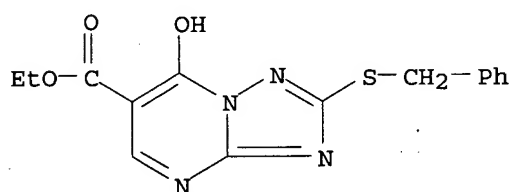
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-(methylthio)- (9CI) (CA INDEX NAME)

INDEX NAME)



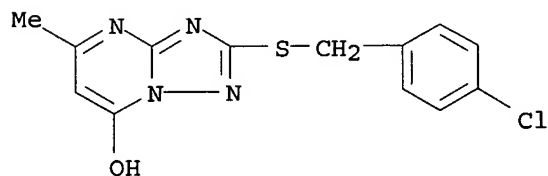
RN 51646-43-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-hydroxy-2-[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



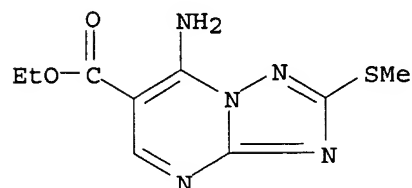
RN 56347-20-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[[4-(4-chlorophenyl)methyl]thio]-5-methyl- (9CI) (CA INDEX NAME)



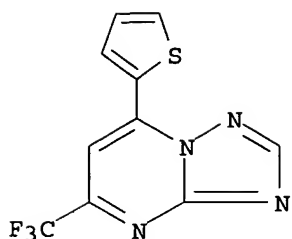
RN 90559-98-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)-, ethyl ester (9CI) (CA INDEX NAME)

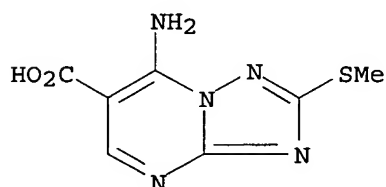


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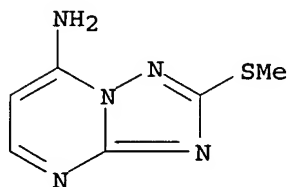
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(2-thienyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



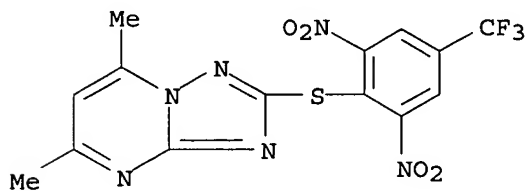
RN 113967-71-8 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)-  
 (9CI) (CA INDEX NAME)



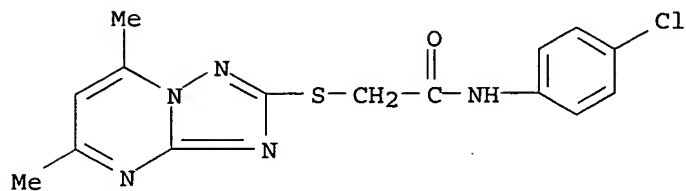
RN 113967-74-1 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 2-(methylthio)- (9CI) (CA INDEX  
 NAME)



RN 194342-06-8 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[2,6-dinitro-4-(trifluoromethyl)phenyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)

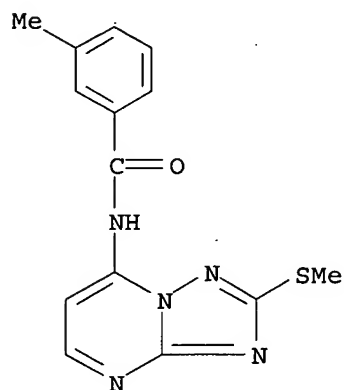


RN 212074-47-0 HCAPLUS  
 CN Acetamide, N-(4-chlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)



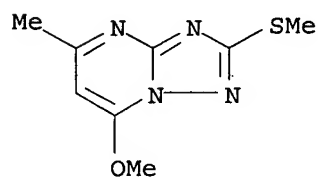
RN 244167-89-3 HCAPLUS

CN Benzamide, 3-methyl-N-[2-(methylthio)[1,2,4]triazolo[1,5-a]pyrimidin-7-yl]-(9CI) (CA INDEX NAME)



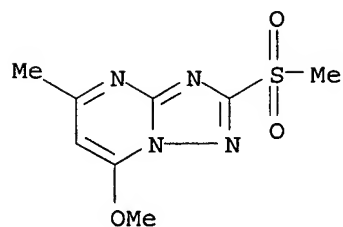
RN 245082-87-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylthio)-(9CI) (CA INDEX NAME)



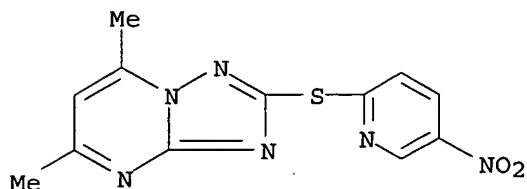
RN 245413-82-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylsulfonyl)-(9CI) (CA INDEX NAME)



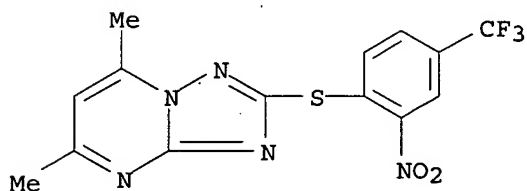
RN 261704-08-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(5-nitro-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)



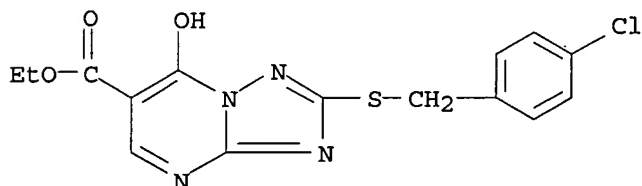
RN 261704-09-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[[2-nitro-4-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



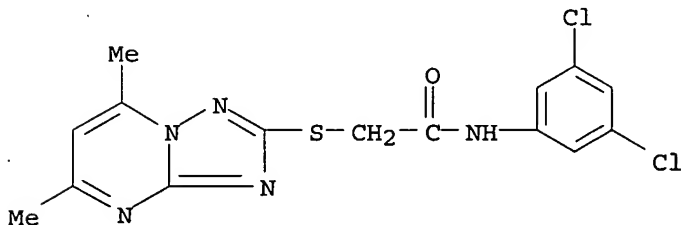
RN 262291-81-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 2-[[[4-chlorophenyl)methyl]thio]-7-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



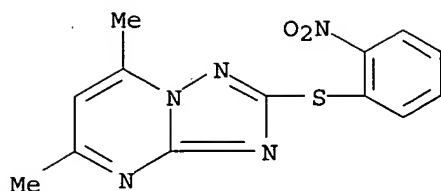
RN 263267-38-5 HCAPLUS

CN Acetamide, N-(3,5-dichlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)

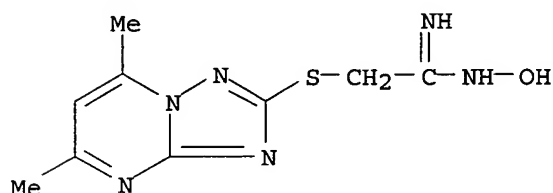


RN 287728-46-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



RN 645337-21-9 HCAPLUS  
 CN Ethanimidamide, 2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]-N-hydroxy- (9CI) (CA INDEX NAME)



L24 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2004:20322 HCAPLUS  
 DOCUMENT NUMBER: 140:87658  
 TITLE: Peptidomimetic modulators of cell adhesion  
 INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shaomeng; Hu, Zengjian  
 PATENT ASSIGNEE(S): Can.  
 SOURCE: U.S. Pat. Appl. Publ., 280 pp., Cont.-in-part of U.S. Ser. No. 6,982.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 14  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE        |
|------------------------|------|----------|-----------------|-------------|
| US 2004006011          | A1   | 20040108 | US 2003-425557  | 20030428    |
| US 6031072             | A    | 20000229 | US 1997-893534  | 19970711    |
| US 6326352             | B1   | 20011204 | US 2000-507102  | 20000217    |
| US 2002168761          | A1   | 20021114 | US 2001-769145  | 20010124    |
| US 2002151475          | A1   | 20021017 | US 2001-6982    | 20011204    |
| PRIORITY APPLN. INFO.: |      |          | US 1996-21612P  | P 19960712  |
|                        |      |          | US 1997-893534  | A1 19970711 |
|                        |      |          | US 2000-491078  | B2 20000124 |
|                        |      |          | US 2000-507102  | A1 20000217 |
|                        |      |          | US 2001-769145  | B2 20010124 |
|                        |      |          | US 2001-6982    | A2 20011204 |

OTHER SOURCE(S): MARPAT 140:87658  
 AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a

three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM A61K038-00

NCL 514009000

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT 57-88-5D, Cholest-5-en-3-ol (3 $\beta$ )-, glycoside derivs. 135-16-0,  
L-Glutamic acid, N-[4-[(2-amino-1,4,5,6,7,8-hexahydro-4-oxo-6-  
pteridiny]methyl]amino]benzoyl]- 487-49-0, Ethanone,  
1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- 548-73-2,  
2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-  
tetrahydro-4-pyridinyl]-1,3-dihydro- 570-88-7, Cholest-4-ene-3,6-diol,  
(3 $\beta$ ,6 $\beta$ )- 1210-66-8, 1H-Purin-6-amine, N-phenyl- 1482-74-2,  
2-Propen-1-one, 3-phenyl-1-(2,3,4-trihydroxyphenyl)- 1699-40-7,  
Benzeneacetamide, 4-methoxy-N-[2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]-  
3-(phenylmethoxy)- 1776-30-3, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-  
phenyl- 2486-02-4, Benzoic acid, 3,4,5-trihydroxy-, 3-methylbutyl ester  
2810-37-9, 1H-Isoindole-1,3(2H)-dione, 2-[5-(1H-benzotriazol-1-yl)propyl]-  
2979-51-3, 1H-Imidazole, 1-(1-oxo-3-phenyl-2-propenyl)- 3242-68-0,  
L-Glutamic acid, N-[4-[[2-[(2-amino-1,4-dihydro-4-oxo-5-  
pyrimidinyl)amino]ethyl]amino]benzoyl]- 3257-73-6, 9H-Purin-6-amine,  
9-[2,3,5-tris-O-(phenylmethyl)- $\beta$ -D-arabinofuranosyl]- 3561-56-6,  
L-Asparagine, N2-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester  
3566-25-4, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-  
pteridiny]ethyl]amino]benzoyl]- 3575-07-3, 1H-Benzimidazole,  
2,2'-(1,2-ethanediyl)bis- 3922-47-2, 1H-1,2,4-Triazol-3-amine,  
5-[(phenylmethyl)thio]- 4672-96-2, Benzeneacetamide,  
3-methoxy-N-[2-[4-methoxy-3-(phenylmethoxy)phenyl]ethyl]-4-(phenylmethoxy)-  
5226-71-1, Benzene, 1,1'-[1,10-decanediylbis(oxy)]bis[3-nitro-  
5341-00-4, 1,4-Naphthalenedione, 2-[3-(decahydro-2-naphthalenyl)propyl]-3-  
hydroxy- 5415-88-3, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-  
(4-phenylbutoxy)- 5421-95-4, Urea, (3-phenyl-1,2,4-oxadiazol-5-yl)-  
5426-87-9, Benzamide, N-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-  
purin-8-yl)methyl]- 5429-46-9, Benzamide, N-[2-(2,3,6,7-tetrahydro-1,3-  
dimethyl-2,6-dioxo-1H-purin-8-yl)ethyl]- 5446-36-6, 1H-Purin-6-amine,  
N-(4-methylphenyl)- 5454-50-2, Ethanone, 1-phenyl-2-(1H-purin-6-ylthio)-  
5454-52-4, 1H-Purine, 6-[(2-phenoxyethyl)thio]- 5508-58-7,  
2(3H)-Furanone, 3-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-  
(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydr  
o-4-hydroxy-, (3E,4S)- 5534-95-2 5800-34-0, Pentanoic acid,  
5-[[[(1S)-2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]-5-oxo-  
6286-57-3, 5(4H)-Isoxazolone, 4-(1,3-benzodioxol-5-ylmethylene)-3-  
phenyl- 6295-27-8, 7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one,  
5-amino-2,6-dihydro-2-phenyl- 6300-80-7, Benzaldehyde,  
4-(dimethylamino)-, 7H-purin-6-ylhydrazone 6320-71-4,  
1,4-Naphthalenedione, 2-(4-cyclohexylbutyl)-3-hydroxy- 6322-09-4,  
2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]-7-methyl- 6323-88-2,  
2(1H)-Quinoxalinone, 3-[2-(3-nitrophenyl)ethenyl]- 6323-89-3,  
2(1H)-Quinoxalinone, 3-(2-phenylethenyl)- 6331-03-9, Benzaldehyde,  
4-nitro-, 7H-purin-6-ylhydrazone 6338-84-7, 1H-Purine-2,6-dione,  
3,7-dihydro-1,3,7-trimethyl-8-(2-phenylethyl)- 6340-76-7,  
2,4-Pyrimidinediamine, 6-chloro-N4-(3-methylphenyl)- 6633-66-5,  
2,4,6-Pyrimidinetriamine, N4-(4-bromophenyl)- 6807-82-5, L-Glutamic  
acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-pteridiny]methyl]amino]benzoyl]-  
L- $\alpha$ -glutamyl- 6962-62-5, 2-Propen-1-one, 3-(1,3-benzodioxol-5-yl)-  
1-(2,4-dihydroxyphenyl)- 6975-34-4, 1H-Purine, 6-[(3-phenyl-2-  
propenyl)thio]- 7781-29-5, 2,4-Pyrimidinediamine, 6-methyl-N4-phenyl-

10320-97-5, 1,2,3,4-Thiatriazol-5-amine, N-1-naphthalenyl- 13184-14-0,  
 L-Lysine, L-lysyl-L-lysyl- 13351-10-5, 2-Propen-1-one,  
 1-(2,4-dihydroxyphenyl)-3-(4-methoxyphenyl)- 13745-20-5, 2-Propen-1-one,  
 1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)- 15013-60-2,  
 Cholest-4-ene-3,6-diol, (3 $\beta$ ,6 $\alpha$ )- 15970-42-0,  
 1H-Imidazole-1,2-diamine, 4-(4-chlorophenyl)- 16856-21-6, L-Tryptophan,  
 N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-, methyl ester  
 16879-84-8, L-Threonine, N-[(phenylmethoxy)carbonyl]-,  
 (4-nitrophenyl)methyl ester 17357-75-4, 1H-1,2,4-Triazole,  
 3-[[[(4-methoxyphenyl)methyl]thio]- 17430-65-8, L-Tryptophan,  
 N-[(phenylmethoxy)carbonyl]-L-valyl-, methyl ester 17496-31-0,  
 1H-Imidazole, 4-[[[(phenylmethyl)thio]methyl]- 18100-11-3,  
 1,4-Naphthalenedione, 2-(3-cyclohexylbutyl)-3-hydroxy- 18100-12-4,  
 1,4-Naphthalenedione, 2-[3-(4-chlorophenyl)propyl]-3-hydroxy-  
 18211-37-5, 1,4-Naphthalenedione, 2-hydroxy-3-[3-(4-methylphenyl)propyl]-  
 19312-13-1, 2-Propen-1-one, 1-(2,5-dihydroxyphenyl)-3-phenyl-  
 19484-75-4D, 2H-1-Benzopyran-2-one, 3,4-dihydro-7-hydroxy-4-methyl-,  
 furanoside derivative 19889-31-7, 1H-Imidazole-4-propanamide,  
 $\alpha$ -amino-N-2-naphthalenyl- 20621-49-2, 2-Propen-1-one,  
 1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)- 20711-05-1,  
 L-Glutamic acid, N-[4-[[2-(2-amino-1,5,6,7-tetrahydro-4-hydroxy-6-  
 pteridiny]ethyl)amino]benzoyl]- 21108-76-9, Imidazo[2,1-b]thiazol-3(2H)-  
 one, 5,6-dihydro-2-(3-phenyl-2-propenylidene)- 21658-45-7, Glycine,  
 L-arginyl-L-prolyl-L-prolyl- 23567-67-1, Phenol, 4-(1,2,3,4-thiatriazol-  
 5-ylamino)- 23815-88-5, 1-6-Bradykinin 24205-32-1, L-Glutamic acid,  
 N-[4-[[2-(2,4-diamino-5-methyl-6-quinazolinyl)methyl]amino]benzoyl]-  
 , diethylester 24386-39-8, Urea, N-1-naphthalenyl-N'-2-pyrimidinyl-  
 24829-12-7, Phenol, 2-[(1H-1,2,4-triazol-3-ylimino)methyl]- 26962-50-5,  
 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)- 27069-81-4,  
 L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-  
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 4,6(1H,5H)-Pyrimidinedione, 5-[[4-(dimethylamino)phenyl]methylene]dihydro-  
 2-thioxo- 27430-17-7, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-phenyl-2-  
 propenylidene)-2-thioxo- 28005-33-6, Benzene, 1,1'-methylenebis[4-[(4-  
 nitrophenyl)thio]- 28246-23-3, Ethanone, 2-(1H-imidazol-2-ylthio)-1-  
 phenyl- 28772-56-7, 2H-1-Benzopyran-2-one, 3-[3-(4'-bromo[1,1'-biphenyl]-  
 4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxy- 29654-52-2, Benzene,  
 1,1'-methylenebis[4-[(4-nitrophenyl)sulfonyl]- 30148-18-6, Methanone,  
 (4-chlorophenyl)(1-methyl-1H-imidazol-2-yl)- 30216-31-0D, Benzoxazole,  
 2-[2-(2-chlorophenyl)ethenyl]-, derivs. 30355-60-3, 1,3,5-Triazine-2,4-  
 diamine, 6-(chloromethyl)-N-phenyl- 30826-46-1, L-Glutamic acid,  
 N-[4-[[[5,7-bis(acetylamino)pyrido[3,4-b]pyrazin-3-  
 yl]methyl]methylamino]benzoyl]-, diethyl ester 30826-47-2, L-Glutamic  
 acid, N-[4-[[[6,8-bis(acetylamino)pyrido[2,3-b]pyrazin-2-  
 yl]methyl]methylamino]benzoyl]-, diethyl ester 33254-46-5,  
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 1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-3-ylthio)- 40538-65-6,  
 5(4H)-Isoxazolone, 3-methyl-4-[(phenylamino)methylene]- 40816-36-2,  
 4,6-Pyrimidinediamine, 5-nitro-N-phenyl- 41266-78-8,  
 1H-1,2,4-Triazol-3-amine, 5-[[[(4-chlorophenyl)methyl]thio]- 41600-13-9,  
 L-Glutamic acid, N-[4-[[[2-(2,4-diamino-6-pteridiny]methyl]methylamino]benzo  
 yl]-L- $\gamma$ -glutamyl- 42220-83-7, 2-Propen-1-one, 1-(2,4-  
 dihydroxyphenyl)-3-(3-hydroxyphenyl)- 46825-86-9, Pyrimidinetetramine,  
 N4-(4-bromophenyl)- 50602-77-2, L-Glutamic acid, N-[4-[[[2-(2,4-diamino-6-  
 pteridiny]methyl]methylamino]benzoyl]-, dibutyl ester 51646-15-2  
 , [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-  
 51893-98-2, Benzoic acid, 2-hydroxy-, [2-[(5-ethyl-1,4-dihydro-6-methyl-4-  
 oxo-2-pyrimidinyl)thio]-1-phenylethylidene]hydrazide 51934-26-0,

L-Glutamic acid, N-[4-[[[(7-amino-1,5-dihydro-5-thioxopyrimido[5,4-e]-1,2,4-triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester, monohydrochloride  
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 2-Propen-1-one, 1-(2,4-dihydroxy-3,6-dimethoxyphenyl)-3-phenyl-  
 54395-52-7, 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis[2-methyl- 56025-86-6, 1H-Purine-2,6-dione,  
 3,7-dihydro-3-methyl-7-(phenylmethyl)- 56307-99-4, Ethanone,  
 1-(2,4-dihydroxyphenyl)-2-(phenylthio)- 57710-80-2, 1H-Benzotriazole-1-carboxylic acid, phenylmethyl ester 57808-66-9, 2H-Benzimidazol-2-one,  
 5-chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-piperidinyll]-1,3-dihydro- 57966-42-4, L-Threonine, L-arginyl-L-tyrosyl-L-leucyl-L-prolyl- 58677-09-1, L-Glutamic acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)methyl]methylamino]benzoyl]-, diethyl ester  
 60045-61-6, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-[(4-methoxyphenyl)methylene]-2-thioxo- 60407-48-9, L-Isoleucine,  
 L-arginylglycyl-L-prolyl-L-phenylalanyl-L-prolyl- 60482-96-4, L-Leucine,  
 L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 61043-53-6,  
 L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-N-(4-nitrophenyl)- 64792-21-8, 2-Propenal, 3-phenyl-, (1,4-dihydro-6-methyl-4-oxo-2-pyrimidinyl)hydrazone 64801-58-7, L-Aspartic acid,  
 N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-γ-glutamyl- 65147-09-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucylglycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 65757-04-2,  
 L-Glutamic acid, N-[4-[[[(1,2,3,4-tetrahydro-2-imino-1,3-dimethyl-4-oxo-6-pteridinyll)methyl]amino]benzoyl]-, dimethyl ester 65757-05-3, L-Glutamic acid, N-[4-[[[(2-amino-3,4-dihydro-3-methyl-4-oxo-6-pteridinyll)methyl]amino]benzoyl]-, dimethyl ester 65877-43-2D,  
 1,3-Benzenediol, 5-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]-, glycoside derivative 66048-53-1, Guanosine, 2',3',5'-tribenzoate 66147-31-7,  
 L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-, 5-butyl ester 67368-29-0, L-Alanine, L-methionyl-L-arginyl-L-phenylalanyl- 67655-19-0, Phenol, 2,2'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis- 67836-16-2, Acetamide, 2-(2,4-dichlorophenoxy)-N-1H-1,2,4-triazol-3-yl- 68047-41-6, 1,3,4-Oxadiazole,  
 2-(3-bromophenyl)-5-(2-naphthalenyl)- 68215-68-9, Phenol,  
 2-[4-amino-6-[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-4-chloro-68682-02-0, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)- 68838-40-4, 1H-1,2,4-Triazole,  
 3-methyl-5-[(phenylmethyl)thio]- 69097-98-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- 69193-20-0,  
 4-Pyrimidinamine, 5-bromo-N-phenyl- 69480-15-5, 3H-1,2,4-Triazole-3-thione, 5-[4-(1,1-dimethylethyl)phenyl]-1,2-dihydro- 70280-72-7,  
 L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridinyll)methyl] (phenylmethyl)amino]benzoyl]-, diethyl ester 70280-75-0, L-Glutamic acid,  
 N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]ethylamino]benzoyl]-, diethyl ester 70539-54-7, L-Glutamic acid, N-[3,5-dichloro-4-[[[(2,4-diamino-6-pteridinyll)methyl]ethylamino]benzoyl]-, diethyl ester 70968-04-6,  
 L-Leucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)- 71047-38-6, 1H-Imidazole, 1-(3,7-dimethyl-2,6-octadienyl)-71074-46-9, Glycine, N-[N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-γ-glutamyl]- 71074-48-1,  
 L-Aspartic acid, N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-α-glutamyl- 71074-49-2, L-Glutamic acid,  
 N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-α-glutamyl- 71707-02-3, L-Glutamic acid, N-[N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]amino]benzoyl]-L-γ-glutamyl]- 72630-15-0,  
 Glutamic acid, N-[4-[[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridinyll)ethyl]amino]benzoyl]- 72682-77-0, L-Isoleucinamide,

N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)-  
 72704-76-8, 2-Propen-1-one, 3-(3,4-dihydroxyphenyl)-1-phenyl-  
 73554-90-2, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-  
 phenylalanyl-L-seryl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-  
 73572-58-4, L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-L-  
 phenylalanyl-L-leucyl-L-phenylalanyl-L-leucyl- 74039-67-1,  
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(3-phenyl-2-propenyl)-  
 74405-42-8, Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-  
 2'-deoxy-, 3'-(hydrogen butanedioate) 74405-44-0, Cytidine,  
 N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen  
 butanedioate) 74853-69-3, L-Leucine, N2-acetyl-L-arginyl-L-arginyl-L-  
 prolyl-L-tyrosyl-L-isoleucyl- 75651-68-2, L-Phenylalaninamide,  
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-prolyl-N-(4-nitrophenyl)-  
 75960-43-9, 1H-Imidazole-4-hexanoic acid, 5-(chloromethyl)-2,3-dihydro-  
 8,2-dioxo-, ethyl ester 76172-68-4, 1-Propanone,  
 3-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- 80032-99-1,  
 1H-1,2,4-Triazole, 3,3'-[1,4-butanediylbis(thio)]bis- 80360-08-3,  
 L-Glutamic acid, N-[4-[[[2,4-diaminopyrido[2,3-d]pyrimidin-6-  
 yl)methyl]amino]benzoyl]-, diethylester 81066-61-7, 2-Pyridinamine,  
 3-[[4-(1,1-dimethylethyl)phenyl]methoxy]- 81587-37-3, 3-Pyridinethiol,  
 2-[(2,6-diamino-4-pyrimidinyl)amino]-6-methyl- 82628-82-8, 1-Propanone,  
 3-(4-nitrophenyl)-1-(2,4,6-trihydroxyphenyl)- 82855-85-4, L-Glutamic  
 acid, N-[4-[[[2-amino-1,4,5,6,7,8-hexahydro-4-oxopyrido[3,2-d]pyrimidin-6-  
 yl)methyl]amino]benzoyl]-, diethyl ester 85122-85-6,  
 1H-Isoindole-1,3(2H)-dione, 2,2'-[1,3-propanediylbis(4,1-  
 piperidinediylmethylene)]bis- 86669-33-2, L-Glutamic acid,  
 N-[4-[[[2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-,  
 bis(1,1-dimethylethyl) ester 90259-60-2, Benzamide, 2-amino-N-[3-(1H-  
 imidazol-1-yl)propyl]- 90259-61-3, Benzamide, 2-[[[4-  
 chlorophenyl)sulfonyl]amino]-N-[3-(1H-imidazol-1-yl)propyl]- 92899-39-3,  
 Glycine, L-valylglycyl-L-valyl-L-alanyl-L-prolyl- 92954-99-9, Glycine,  
 1-acetyl-L-prolyl-L-leucylglycyl-L-leucyl-L-leucyl-, ethyl ester  
 93515-01-6, L-Threonine, L-tyrosyl-L-prolyl-L-prolyl-L- $\alpha$ -glutamyl-L-  
 prolyl-L- $\alpha$ -glutamyl- 93524-30-2,  $\beta$ -D-Glucopyranosiduronic  
 acid, (3 $\alpha$ ,5 $\beta$ )-21-(acetyloxy)-20-[(aminocarbonyl)hydrazono]pregn  
 an-3-yl, methyl ester, 2,3,4-triacetate 93674-97-6, L-Serine,  
 L-arginylglycyl-L- $\alpha$ -glutamyl- 95192-21-5, L-Phenylalaninamide,  
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-alanyl-N-(4-nitrophenyl)-  
 95192-38-4, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-  
 valyl-L-prolyl-N-(4-nitrophenyl)- 95210-75-6, L-Proline,  
 L-tyrosyl-L-prolyl-L-phenylalanyl-L-valyl-L- $\alpha$ -glutamyl-L-prolyl-L-  
 isoleucyl- 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-  
 phenyl- 98151-93-0, L-Proline, L-tyrosyl-L-prolyl-L-phenylalanyl-L-  
 prolylglycyl-L-prolyl-L-isoleucyl- 100975-56-2, Benzaldehyde,  
 4-hydroxy-, (2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-  
 yl)hydrazone 102212-40-8, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-  
 8-[(2-phenylethyl)amino]- 103030-49-5, 2,4-Pyrimidinediamine,  
 N4-(4-chlorophenyl)-5-nitro- 103398-43-2, Benzenemethanol,  
 2-[bis[2-[(4-nitrobenzoyl)oxy]ethyl]amino]-, 4-nitrobenzoate (ester)  
 105037-36-3, Benzenesulfonic acid, 4-[(7-chloro-4-quinazolinyl)amino]-  
 108608-63-5, Glycine, L-seryl-L- $\alpha$ -aspartylglycyl-L-arginyl-  
 110906-89-3, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-  
 L-alanyl-L-alanyl-N-(4-nitrophenyl)- 111172-14-6, 1,3-Benzodioxole-5-  
 carboxaldehyde, O-(2-thienylcarbonyl)oxime 112233-74-6, Carbamic acid,  
 diphenyl-, 2-(acetyl amino)-1H-purin-6-yl ester 113866-00-5,  
 L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L-  
 prolyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl ester  
 113866-16-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -  
 glutamyl-L-alanyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl

ester 117889-48-2, 1H-Tetrazole, 5-[(2,4-dichlorophenoxy)methyl]-  
 118034-92-7, L-Threonine, L-histidyl-L-phenylalanyl-L-methionyl-L-prolyl-  
 120225-54-9, Benzenepropanoic acid, 4-[2-[[6-amino-9-(N-ethyl-β-D-  
 ribofuranuronamidosyl)-9H-purin-2-yl]amino]ethyl]- 121036-80-4,  
 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methylphenyl)ethenyl]-3-phenyl-  
 121036-81-5, 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methoxyphenyl)ethenyl]-3-  
 phenyl- 124485-41-2, L-Argininamide, N-[(phenylmethoxy)carbonyl]-L-valyl-  
 L-valyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 126235-09-4,  
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-phenylethyl)-  
 128802-79-9, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-  
 isoleucyl-L-prolyl-N-(4-nitrophenyl)- 131061-65-9, 7H-Purine-7-butanoic  
 acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-[(phenylmethyl)amino]-,  
 ethyl ester 132467-01-7, 2(1H)-Quinoxalinone, 3-[2-(2-  
 chlorophenyl)ethenyl]- 133061-57-1, 2,4-Pyrimidinediamine,  
 N4-(3,5-dichlorophenyl)-6-methyl- 134759-22-1, 1H-Thieno[3,4-d]imidazole-  
 4-pentanamide, N-[6-[[5-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-  
 1(3H),9']-[9H]xanthen]-5-yl]amino]thioxomethyl]amino]pentyl]amino]-6-  
 oxohexyl]hexahydro-2-oxo-, (3aS,4S,6aR)- 134796-34-2, 1H-1,2,4-Triazole,  
 3-[[4-(chlorophenyl)methyl]thio]- 137484-84-5  
 , 1,3,5-Triazin-2-amine, 4-chloro-6-[3-(2-furanyl)propoxy]-N,N-dimethyl-  
 137833-31-9, Myelo peptide 2 138194-56-6, 1H-Pyrrole-2,5-dione,  
 1-[3-[[4-(4-oxo-1,2,3-benzotriazin-3(4H)-yl)oxy]carbonyl]phenyl]-  
 138915-75-0, L-Leucine, N-acetyl-L-histidyl-L-tryptophyl-L-alanyl-L-  
 valylglycyl-L-histidyl- 142206-40-4, 1H-Benzimidazole,  
 2,2'-(1,3-propanediyl)bis[1-methyl- 143113-41-1, L-Valine,  
 L-Histidyl-L-Alanyl 146871-70-7, 4-Quinazolinamine, N-(3-chlorophenyl)-,  
 monohydrochloride 148337-06-8, Glycine, L-prolylglycyl-L-alanyl-L-  
 isoleucyl-L-prolyl- 151358-70-2, 2-Propen-1-one, 1,1'-(2,6-  
 pyridinediyl)bis[3-(4-hydroxyphenyl)- 152028-96-1, 1H-Imidazole,  
 4-[3-[[4-(iodophenyl)methoxy]propyl]- 154719-25-2, L-Lysinamide,  
 N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-  
 dimethylbenzoyl)oxy]-2-oxopropyl]-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-  
 thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]- 155373-59-4,  
 4H-1-Benzopyran-4-one, 3-[[4-(1H-tetrazol-5-yl)phenyl]methyl]-  
 155373-72-1, 4H-1-Benzopyran-4-one, 2-phenyl-7-[4-(1H-tetrazol-5-  
 yl)butoxy]- 160347-57-9D, 2(1H)-Pyrimidinone, 5-(4-pentylphenyl)-,  
 derivs. 185503-97-3, L-Lysine, N6-[[4-[[4-(dimethylamino)phenyl]azo]phen-  
 yl]sulfonyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- 188966-22-5D,  
 Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylhexyl)-, derivs.  
 191411-47-9, 1H-Imidazole-5-methanol, 1-methyl-2-[(phenylmethyl)thio]-  
 194424-08-3, Glutamic acid, N-[4-[[3-(2-thienyl)-2-  
 quinoxaliny]amino]benzoyl]-, dipropyl ester 195140-70-6, 1H-Imidazole,  
 1-[2-(phenylmethoxy)ethyl]- 196600-87-0, Tyrosine, N-  
 [(phenylmethoxy)carbonyl]norvalylglycyl-, methyl ester 197456-56-7,  
 1,4-Naphthalenedione, 2-[4-(decahydro-2-naphthalenyl)butyl]-3-hydroxy-  
 198488-04-9, Urea, N,N'-(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis[N'-(2-  
 methylphenyl)- 198632-08-5, L-Proline, glycyl-L-arginylglycyl-L-α-  
 glutamyl-L-threonyl- 199929-21-0, 1,4-Naphthalenedione,  
 2-hydroxy-3-[8-(4-methylphenoxy)octyl]- 200058-34-0,  
 1,4-Naphthalenedione, 2-(3-[1,1'-bicyclohexyl]-4-ylpropyl)-3-hydroxy-  
 200061-22-9, Phenol, 4,4'-(1-methylethylidene)bis-, bis(3,5-  
 dinitrobenzoate) 200431-98-7, 3-Pyridinemethanamine,  
 N-1H-1,2,4-triazol-3-yl- 200505-51-7, Decanedioic acid,  
 bis[[4-(ethoxy-3-methoxyphenyl)methylene]hydrazide] 200706-30-5,  
 4H-1,2,4-Triazol-4-amine, N-[(2,3-dihydro-1H-inden-5-yl)methylene]-  
 200706-45-2, 4-Imidazolidinone, 5-[(2,3-dihydro-1H-inden-5-yl)methylene]-2-  
 thioxo- 201997-13-9, 1,3-Benzenediol, 4-[[[2-hydroxy-2-(4-  
 nitrophenyl)ethyl]imino]methyl]- 202118-27-2, 1H-1,2,4-Triazol-3-amine,  
 N-[(2-iodophenyl)methylene]- 202118-28-3, 1H-1,2,4-Triazol-3-amine,

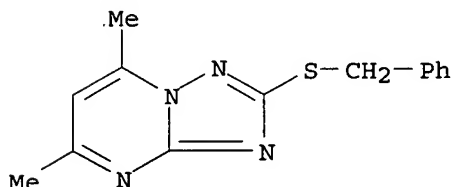
N-[(2-chlorophenyl)methylene]- 202332-09-0, 1,4-Benzenediol,  
 2-(6-methylheptyl)- 202528-15-2, Cyclo(L-alanyl-L-histidyl-L-alanyl-L-  
 valyl-L- $\alpha$ -aspartyl-L-isoleucyl) 206360-24-9, 4H-1-Benzopyran-4-  
 one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-3-(3-methyl-2-butenyl)-  
 210709-22-1, L-Alanine, N2-benzoyl-L-arginyl-L-phenylalanyl-  
 215434-58-5, 1-Piperazinecarbothioamide, N-3-pyridinyl-4-[4-  
 (trifluoromethyl)-2-pyrimidinyl]- 215655-36-0, Benzoic acid,  
 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]-  
 215657-86-6, 2-Pyrrolidinone, 1-[2-hydroxy-3-[4-[4-(trifluoromethyl)-2-  
 pyrimidinyl]-1-piperazinyl]propyl]- 216299-43-3, 2,5-Pyrrolidinedione,  
 1-[[11-[(5-azido-1-naphthalenyl)oxy]-1-oxoundecyl]oxy]-  
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
 PRP (Properties); THU (Therapeutic use); BIOL (Biological study)  
 ; USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion  
 for therapeutic use in relation to three-dimensional structure)

IT 51646-15-2, [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-  
 [(phenylmethyl)thio]-  
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
 PRP (Properties); THU (Therapeutic use); BIOL (Biological study)  
 ; USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion  
 for therapeutic use in relation to three-dimensional structure)

RN 51646-15-2 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-  
 (9CI) (CA INDEX NAME)



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TITLE: Preparation of fused succinimides as modulators of  
 nuclear hormone receptor function

INVENTOR(S): Salvati, Mark E.; Balog, James Aaron; Pickering,  
 Darcia A.; Giese, Soren; Fura, Aberra; Li, Wenying;  
 Patel, Ramesh N.; Hanson, Ronald L.; Mitt, Toomas;  
 Roberge, Jacques; Corte, James R.; Spergel, Steven H.;  
 Rampulla, Richard A.; Misra, Raj; Xiao, Hai-yun

PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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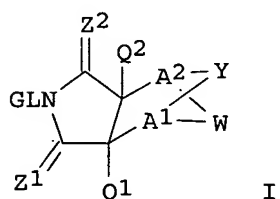
US 2001-25116

A 20011219

OTHER SOURCE(S):

MARPAT 139:164784

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AB Title compds. [I; G = (substituted) aryl, heterocyclyl; Z1, Z2 = O, S, NH, NR6; A1, A2 = CR7, N; Y = JJ'J"; J, J' = (CR7R7')n; n = 0-3, J' = bond, O, S, SO, SO2, NH, NR7, CR7R7', R2PO, R2PS, R2OPO, R2NHPO, OPOOR2, OPONHR2, OSO2, NHNH, NHNR6, NR6NH, N:N, (substituted) cycloalk(en)yl, heterocyclo; W' = CR7R7'CR7R7, CR7R7'CO, COCO, CR7R7'C:CH2, C:CH2C:CH2, CR7R7C:NR1, C:NR1C:NR1, NR9CR7R7, N:N, (substituted) cycloalk(en)yl, heterocyclo, aryl, etc.; Q1, Q2 = H, (substituted) alkyl, alkenyl, cycloalk(en)yl, heterocycloalkyl, aryl(alkyl), alkynyl, heterocyclo, halo, CN, R1O2C, R4CO, R5R6NCO, HOCR7R7', NO2, R1OCH2, R1O, NH2, COSR1, SO2R1, NR4R5; L = bond, (CR7R7')n, NH, NR5, NH(CR7R7')n, NR5(CR7R7')n; R1, R1' = H, R2; R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalk(en)yl, heterocyclo, cycloalk(en)ylalkyl, heterocycloalkyl, aryl(alkyl); R3, R3' = R1, halo, CN, hydroxylamine, hydroxamide, (substituted) alkoxy, alkylthio, amino, NR1R2, SH; R4 = R1, R1CO, R1O2C, R1NHCO, SO2OR1, SO2R1, SO2NR1R1'; R5 = R2, R1CO, R1NHCO, SO2R1, SO2OR1, SO2NR1R1'; R6 = R5, CN, OH, OR1; R7, R7' = R4, halo, CN, OR4, NO2, hydroxylamine, hydroxylamide, amino, NHR4, NR2R5, NR5R5, NOR1, SH, (substituted) alkylthio, HO2C, R1CO2, NH2CO, SOR1, PO3R1R1', R1R1'NCO, COSR1; with provisos], were prepared as modulators of nuclear hormone receptor function (no data). Thus, 4-(tert-butyltrimethylsiloxy)-2H-thiopyran (preparation given) and 1-(4-bromo-3-methylphenyl)-1H-pyrrole-2,5-dione (preparation given) were refluxed 5 h in PhMe to give an enol ether intermediate which was stirred with CF3CO2H in CH2Cl2 to give 22% (3 $\alpha$ ,4 $\alpha$ ,7 $\alpha$ ,7 $\alpha$ )-2-(4-bromo-3-methylphenyl)tetrahydro-4,7-ethanothiopyrano[3,4-c]pyrrole-1,3,8(2H,4H)-trione.

IC ICM C07D491-00

ICS A61K031-40

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

|    |              |              |              |              |              |
|----|--------------|--------------|--------------|--------------|--------------|
| IT | 573722-37-9P | 573722-38-0P | 573722-39-1P | 573722-40-4P | 573722-41-5P |
|    | 573722-42-6P | 573722-43-7P | 573722-44-8P | 573722-46-0P | 573722-48-2P |
|    | 573722-49-3P | 573722-50-6P | 573722-51-7P | 573722-52-8P | 573722-53-9P |
|    | 573722-59-5P | 573722-62-0P | 573722-65-3P | 573722-68-6P | 573722-72-2P |

## Ward PCT/US03/21394

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);  
 USES (Uses)

(preparation of fused succinimides as modulators of nuclear hormone receptor function)

IT 573730-33-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);  
 USES (Uses)

(preparation of fused succinimides as modulators of nuclear hormone receptor function)

RN 573730-33-3 HCAPLUS

CN 1-Naphthalenecarbonitrile, 4-[(3aS,4R,7R,7aR)-octahydro-4-methyl-7-[2-[(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-1,3-dioxo-4,7-epoxy-2H-isindol-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

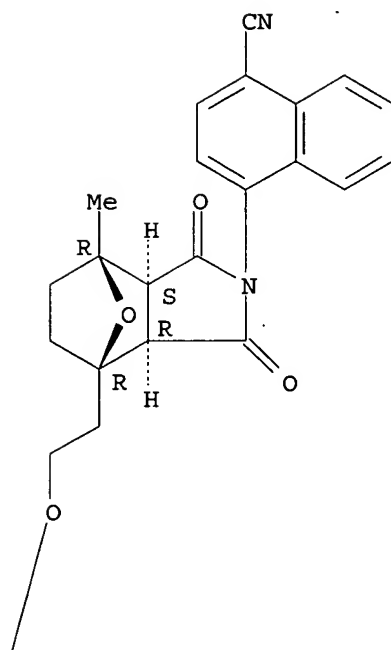
CM 1

CRN 573730-32-2

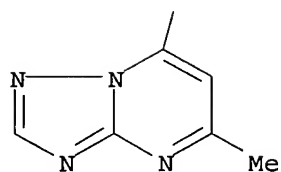
CMF C28 H24 N6 O4

Absolute stereochemistry.

PAGE 1-A



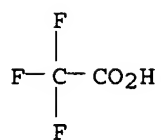
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2002:869496 HCAPLUS  
 DOCUMENT NUMBER: 137:363033  
 TITLE: Peptidomimetic modulators of cell adhesion  
 INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie D.; Wang, Shoameng; Hu, Zenzian  
 PATENT ASSIGNEE(S): Can.  
 SOURCE: U.S. Pat. Appl. Publ., 309 pp., Cont.-in-part of U.S. Ser. No. 491,078.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 14  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE        |
|------------------------|------|----------|-----------------|-------------|
| US 2002168761          | A1   | 20021114 | US 2001-769145  | 20010124    |
| US 2004006011          | A1   | 20040108 | US 2003-425557  | 20030428    |
| PRIORITY APPLN. INFO.: |      |          | US 2000-491078  | A2 20000124 |
|                        |      |          | US 1996-21612P  | P 19960712  |
|                        |      |          | US 1997-893534  | A1 19970711 |
|                        |      |          | US 2000-507102  | A1 20000217 |
|                        |      |          | US 2001-769145  | B2 20010124 |
|                        |      |          | US 2001-6982    | A2 20011204 |

OTHER SOURCE(S): MARPAT 137:363033

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM A61K038-17  
 ICS C07K014-435; C12N005-02

NCL 435325000

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT 57-88-5D, Cholest-5-en-3-ol (3 $\beta$ )-, glycoside derivs. 135-16-0,  
 L-Glutamic acid, N-[4-[(2-amino-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]- 487-49-0, Ethanone,  
 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- 548-73-2,  
 2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-tetrahydro-4-pyridinyl]-1,3-dihydro- 570-88-7, Cholest-4-ene-3,6-diol, (3 $\beta$ ,6 $\beta$ )- 1210-66-8, 1H-Purin-6-amine, N-phenyl- 1482-74-2,  
 2-Propen-1-one, 3-phenyl-1-(2,3,4-trihydroxyphenyl)- 1699-40-7,  
 Benzeneacetamide, 4-methoxy-N-[2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]-3-(phenylmethoxy)- 1776-30-3, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-phenyl- 2486-02-4, Benzoic acid, 3,4,5-trihydroxy-, 3-methylbutyl ester 2810-37-9, 1H-Isoindole-1,3(2H)-dione, 2-[5-(1H-benzotriazol-1-yl)propyl]- 2979-51-3, 1H-Imidazole, 1-(1-oxo-3-phenyl-2-propenyl)- 3242-68-0,  
 L-Glutamic acid, N-[4-[[2-[(2-amino-1,4-dihydro-4-oxo-5-pyrimidinyl)amino]ethyl]amino]benzoyl]- 3257-73-6, 9H-Purin-6-amine, 9-[2,3,5-tris-O-(phenylmethyl)- $\beta$ -D-arabinofuranosyl]- 3561-56-6,  
 L-Asparagine, N2-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester

3566-25-4, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)ethyl]amino]benzoyl]- 3575-07-3, 1H-Benzimidazole, 2,2'-(1,2-ethanediyl)bis- 3922-47-2, 1H-1,2,4-Triazol-3-amine, 5-[(phenylmethyl)thio]- 4672-96-2, Benzeneacetamide, 3-methoxy-N-[2-[4-methoxy-3-(phenylmethoxy)phenyl]ethyl]-4-(phenylmethoxy)- 5226-71-1, Benzene, 1,1'-[1,10-decanediylbis(oxy)]bis[3-nitro- 5341-00-4, 1,4-Naphthalenedione, 2-[3-(decahydro-2-naphthalenyl)propyl]-3-hydroxy- 5415-88-3, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(4-phenylbutoxy)- 5421-95-4, Urea, (3-phenyl-1,2,4-oxadiazol-5-yl)- 5426-87-9, Benzamide, N-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)methyl]- 5429-46-9, Benzamide, N-[2-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)ethyl]- 5446-36-6, 1H-Purin-6-amine, N-(4-methylphenyl)- 5454-50-2, Ethanone, 1-phenyl-2-(1H-purin-6-ylthio)- 5454-52-4, 1H-Purine, 6-[(2-phenoxyethyl)thio]- 5508-58-7, 2(3H)-Furanone, 3-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydro-4-hydroxy-, (3E,4S)- 5534-95-2 5800-34-0, Pentanoic acid, 5-[[[(1S)-2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]-5-oxo- 6286-57-3, 5(4H)-Isoxazolone, 4-(1,3-benzodioxol-5-ylmethylene)-3-phenyl- 6295-27-8, 7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one, 5-amino-2,6-dihydro-2-phenyl- 6300-80-7, Benzaldehyde, 4-(dimethylamino)-, 7H-purin-6-ylhydrazone 6320-71-4, 1,4-Naphthalenedione, 2-(4-cyclohexylbutyl)-3-hydroxy- 6322-09-4, 2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]-7-methyl- 6323-88-2, 2(1H)-Quinoxalinone, 3-[2-(3-nitrophenyl)ethenyl]- 6323-89-3, 2(1H)-Quinoxalinone, 3-(2-phenylethenyl)- 6331-03-9, Benzaldehyde, 4-nitro-, 7H-purin-6-ylhydrazone 6338-84-7, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(2-phenylethyl)- 6340-76-7, 2,4-Pyrimidinediamine, 6-chloro-N4-(3-methylphenyl)- 6633-66-5, 2,4,6-Pyrimidinetriamine, N4-(4-bromophenyl)- 6807-82-5, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-L- $\alpha$ -glutamyl- 6962-62-5, 2-Propen-1-one, 3-(1,3-benzodioxol-5-yl)-1-(2,4-dihydroxyphenyl)- 6975-34-4, 1H-Purine, 6-[(3-phenyl-2-propenyl)thio]- 7781-29-5, 2,4-Pyrimidinediamine, 6-methyl-N4-phenyl- 10320-97-5, 1,2,3,4-Thiatriazol-5-amine, N-1-naphthalenyl- 13184-14-0, L-Lysine, L-lysyl-L-lysyl- 13351-10-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-methoxyphenyl)- 13745-20-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)- 15013-60-2, Cholest-4-ene-3,6-diol, (3 $\beta$ ,6 $\alpha$ )- 15970-42-0, 1H-Imidazole-1,2-diamine, 4-(4-chlorophenyl)- 16856-21-6, L-Tryptophan, N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-, methyl ester 16879-84-8, L-Threonine, N-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester 17357-75-4, 1H-1,2,4-Triazole, 3-[[[(4-methoxyphenyl)methyl]thio]- 17430-65-8, L-Tryptophan, N-[(phenylmethoxy)carbonyl]-L-valyl-, methyl ester 17496-31-0, 1H-Imidazole, 4-[[[(phenylmethyl)thio]methyl]- 18100-11-3, 1,4-Naphthalenedione, 2-(3-cyclohexylbutyl)-3-hydroxy- 18100-12-4, 1,4-Naphthalenedione, 2-[3-(4-chlorophenyl)propyl]-3-hydroxy- 18211-37-5, 1,4-Naphthalenedione, 2-hydroxy-3-[3-(4-methylphenyl)propyl]- 19312-13-1, 2-Propen-1-one, 1-(2,5-dihydroxyphenyl)-3-phenyl- 19484-75-4D, 2H-1-Benzopyran-2-one, 3,4-dihydro-7-hydroxy-4-methyl-, furanoside derivative 19889-31-7, 1H-Imidazole-4-propanamide,  $\alpha$ -amino-N-2-naphthalenyl- 20621-49-2, 2-Propen-1-one, 1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)- 20711-05-1, L-Glutamic acid, N-[4-[[2-(2-amino-1,5,6,7-tetrahydro-4-hydroxy-6-pteridinyl)ethyl]amino]benzoyl]- 21108-76-9, Imidazo[2,1-b]thiazol-3(2H)-one, 5,6-dihydro-2-(3-phenyl-2-propenylidene)- 21658-45-7, Glycine, L-arginyl-L-prolyl-L-prolyl- 23567-67-1, Phenol, 4-(1,2,3,4-thiatriazol-5-ylamino)- 23815-88-5, 1-6-Bradykinin 24205-32-1, L-Glutamic acid,

N-[4-[[[(2,4-diamino-5-methyl-6-quinazolinyl)methyl]amino]benzoyl]-  
 ,diethylester 24386-39-8, Urea, N-1-naphthalenyl-N'-2-pyrimidinyl-  
 24829-12-7, Phenol, 2-[(1H-1,2,4-triazol-3-ylimino)methyl]- 26962-50-5,  
 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)- 27069-81-4,  
 L-Glutamic acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-  
 quinazolinyl)methyl]amino]benzoyl]-, diethyl ester 27430-15-5,  
 4,6(1H,5H)-Pyrimidinedione, 5-[[4-(dimethylamino)phenyl]methylene]dihydro-  
 2-thioxo- 27430-17-7, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-phenyl-2-  
 propenylidene)-2-thioxo- 28005-33-6, Benzene, 1,1'-methylenebis[4-[(4-  
 nitrophenyl)thio]- 28246-23-3, Ethanone, 2-(1H-imidazol-2-ylthio)-1-  
 phenyl- 28772-56-7, 2H-1-Benzopyran-2-one, 3-[3-(4'-bromo[1,1'-biphenyl]-  
 4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxy- 29654-52-2, Benzene,  
 1,1'-methylenebis[4-[(4-nitrophenyl)sulfonyl]- 30148-18-6, Methanone,  
 (4-chlorophenyl)(1-methyl-1H-imidazol-2-yl)- 30216-31-0D, Benzoxazole,  
 2-[2-(2-chlorophenyl)ethenyl]-, derivs. 30355-60-3, 1,3,5-Triazine-2,4-  
 diamine, 6-(chloromethyl)-N-phenyl- 30826-46-1, L-Glutamic acid,  
 N-[4-[[[5,7-bis(acetylamino)pyrido[3,4-b]pyrazin-3-  
 yl]methyl]methylamino]benzoyl]-, diethyl ester 30826-47-2, L-Glutamic  
 acid, N-[4-[[[6,8-bis(acetylamino)pyrido[2,3-b]pyrazin-2-  
 yl]methyl]methylamino]benzoyl]-, diethyl ester 33254-46-5,  
 6H-Purine-6-thione, 1,9-dihydro-9-(3-phenylpropyl)- 34396-76-4,  
 6H-Purin-6-one, 1,9-dihydro-9-(3-phenylpropyl)- 37664-31-6, Ethanone,  
 1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-3-ylthio)- 40538-65-6,  
 5(4H)-Isoxazolone, 3-methyl-4-[(phenylamino)methylene]- 40816-36-2,  
 4,6-Pyrimidinediamine, 5-nitro-N-phenyl- 41266-78-8,  
 1H-1,2,4-Triazol-3-amine, 5-[[[(4-chlorophenyl)methyl]thio]- 41600-13-9,  
 L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzo  
 yl]-L-γ-glutamyl- 42220-83-7, 2-Propen-1-one, 1-(2,4-  
 dihydroxyphenyl)-3-(3-hydroxyphenyl)- 46825-86-9, Pyrimidinetetramine,  
 N4-(4-bromophenyl)- 50602-77-2, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-  
 pteridiny]methyl]methylamino]benzoyl]-, dibutyl ester 51646-15-2\*\*\*,  
 [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-  
 51893-98-2, Benzoic acid, 2-hydroxy-, [2-[(5-ethyl-1,4-dihydro-6-methyl-4-  
 oxo-2-pyrimidinyl)thio]-1-phenylethylidene]hydrazide 51934-26-0,  
 L-Glutamic acid, N-[4-[[[(7-amino-1,5-dihydro-5-thioxopyrimido[5,4-e]-1,2,4-  
 triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester, monohydrochloride  
 51934-28-2, L-Glutamic acid, N-[4-[[[(5,7-diaminopyrimido[5,4-e]-1,2,4-  
 triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester 54299-50-2,  
 2-Propen-1-one, 1-(2,4-dihydroxy-3,6-dimethoxyphenyl)-3-phenyl-  
 54395-52-7, 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-  
 phenyleneoxy)]bis[2-methyl- 56025-86-6, 1H-Purine-2,6-dione,  
 3,7-dihydro-3-methyl-7-(phenylmethyl)- 56307-99-4, Ethanone,  
 1-(2,4-dihydroxyphenyl)-2-(phenylthio)- 57710-80-2, 1H-Benzotriazole-1-  
 carboxylic acid, phenylmethyl ester 57808-66-9, 2H-Benzimidazol-2-one,  
 5-chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-  
 piperidinyl]-1,3-dihydro- 57966-42-4, L-Threonine, L-arginyl-L-tyrosyl-L-  
 leucyl-L-prolyl- 58677-09-1, L-Glutamic acid, N-[4-[[[(2-amino-1,4-  
 dihydro-4-oxo-6-quinazolinyl)methyl]methylamino]benzoyl]-, diethyl ester  
 60045-61-6, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-[(4-  
 methoxyphenyl)methylene]-2-thioxo- 60407-48-9, L-Isoleucine,  
 L-arginylglycyl-L-prolyl-L-phenylalanyl-L-prolyl- 60482-96-4, L-Leucine,  
 L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 61043-53-6,  
 L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-N-(4-  
 nitrophenyl)- 64792-21-8, 2-Propenal, 3-phenyl-, (1,4-dihydro-6-methyl-4-  
 oxo-2-pyrimidinyl)hydrazone 64801-58-7, L-Aspartic acid,  
 N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-γ-  
 glutamyl- 65147-09-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-  
 leucylglycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 65757-04-2,  
 L-Glutamic acid, N-[4-[[[(1,2,3,4-tetrahydro-2-imino-1,3-dimethyl-4-oxo-6-

pteridiny]methyl]amino]benzoyl]-, dimethyl ester 65757-05-3, L-Glutamic acid, N-[4-[[[(2-amino-3,4-dihydro-3-methyl-4-oxo-6-pteridiny]methyl]amino]benzoyl]-, dimethyl ester 65877-43-2D, 1,3-Benzenediol, 5-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]-, glycoside derivative 66048-53-1, Guanosine, 2',3',5'-tribenzoate 66147-31-7, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-, 5-butyl ester 67368-29-0, L-Alanine, L-methionyl-L-arginyl-L-phenylalanyl- 67655-19-0, Phenol, 2,2'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis- 67836-16-2, Acetamide, 2-(2,4-dichlorophenoxy)-N-1H-1,2,4-triazol-3-yl- 68047-41-6, 1,3,4-Oxadiazole, 2-(3-bromophenyl)-5-(2-naphthalenyl)- 68215-68-9, Phenol, 2-[4-amino-6-[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-4-chloro-68682-02-0, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)- 68838-40-4, 1H-1,2,4-Triazole, 3-methyl-5-[(phenylmethyl)thio]- 69097-98-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- 69193-20-0, 4-Pyrimidinamine, 5-bromo-N-phenyl- 69480-15-5, 3H-1,2,4-Triazole-3-thione, 5-[4-(1,1-dimethylethyl)phenyl]-1,2-dihydro- 70280-72-7, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl] (phenylmethyl) amino]benzoyl]-, diethyl ester 70280-75-0, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]ethylamino]benzoyl]-, diethyl ester 70539-54-7, L-Glutamic acid, N-[3,5-dichloro-4-[[[(2,4-diamino-6-pteridiny]methyl]ethylamino]benzoyl]-, diethyl ester 70968-04-6, L-Leucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)- 71047-38-6, 1H-Imidazole, 1-(3,7-dimethyl-2,6-octadienyl)-71074-46-9, Glycine, N-[N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-γ-glutamyl]- 71074-48-1, L-Aspartic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-α-glutamyl- 71074-49-2, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-α-glutamyl- 71707-02-3, L-Glutamic acid, N-[N-[4-[[[(2,4-diamino-6-pteridiny]methyl]amino]benzoyl]-L-γ-glutamyl]- 72630-15-0, Glutamic acid, N-[4-[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridiny]ethyl]amino]benzoyl]- 72682-77-0, L-Isoleucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)-72704-76-8, 2-Propen-1-one, 3-(3,4-dihydroxyphenyl)-1-phenyl-73554-90-2, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-seryl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-73572-58-4, L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-leucyl-L-phenylalanyl-L-leucyl- 74039-67-1, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(3-phenyl-2-propenyl)-74405-42-8, Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen butanedioate) 74405-44-0, Cytidine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen butanedioate) 74853-69-3, L-Leucine, N2-acetyl-L-arginyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 75651-68-2, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-prolyl-N-(4-nitrophenyl)-75960-43-9, 1H-Imidazole-4-hexanoic acid, 5-(chloromethyl)-2,3-dihydro-ε,2-dioxo-, ethyl ester 76172-68-4, 1-Propanone, 3-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- 80032-99-1, 1H-1,2,4-Triazole, 3,3'-[1,4-butanediylbis(thio)]bis- 80360-08-3, L-Glutamic acid, N-[4-[[[(2,4-diaminopyrido[2,3-d]pyrimidin-6-yl)methyl]amino]benzoyl]-, diethyl ester 81066-61-7, 2-Pyridinamine, 3-[[4-(1,1-dimethylethyl)phenyl]methoxy]- 81587-37-3, 3-Pyridinethiol, 2-[(2,6-diamino-4-pyrimidinyl)amino]-6-methyl- 82628-82-8, 1-Propanone, 3-(4-nitrophenyl)-1-(2,4,6-trihydroxyphenyl)- 82855-85-4, L-Glutamic acid, N-[4-[[[(2-amino-1,4,5,6,7,8-hexahydro-4-oxopyrido[3,2-d]pyrimidin-6-yl)methyl]amino]benzoyl]-, diethyl ester 85122-85-6, 1H-Isoindole-1,3(2H)-dione, 2,2'-[1,3-propanediylbis(4,1-

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 128802-79-9, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-  
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 , 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis[1-methyl- 143113-41-1,

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RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); \*\*\*BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

IT 51646-15-2, [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-

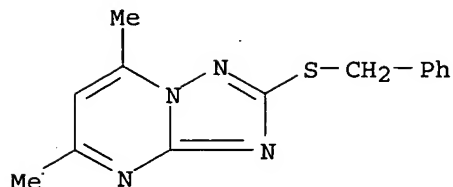
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

RN 51646-15-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-

(9CI) (CA INDEX NAME)



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DOCUMENT NUMBER: 135:147398

TITLE: Peptidomimetic modulators of cell adhesion

INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shoameng; Hu, Zengjian

PATENT ASSIGNEE(S): Adherex Technologies, Inc., Can.

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-491078 A 20000124

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AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM C07K007-00

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT 57-88-5D, Cholest-5-en-3-ol (3 $\beta$ )-, glycoside derivs. 135-16-0

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 160347-57-9D, derivs. 185503-97-3 188966-22-5D, derivs. 191411-47-9  
 194424-08-3 195140-70-6 196600-87-0 197456-56-7 198488-04-9  
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 202118-28-3 202332-09-0 202528-15-2 206360-24-9 210709-22-1  
 215434-58-5 215655-36-0 215657-86-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

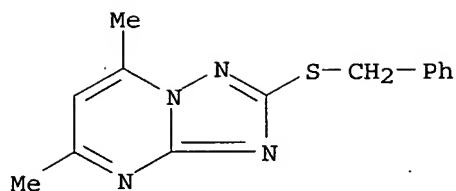
IT 51646-15-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

RN 51646-15-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-(9CI) (CA INDEX NAME)



L24 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:402315 HCAPLUS

DOCUMENT NUMBER: 129:81753

TITLE: Preparation of substituted aryl piperazines as modulators of chemokine receptor activity

INVENTOR(S): Mills, Sander G.; Springer, Martin S.; MacCoss, Malcolm

PATENT ASSIGNEE(S): Merck &amp; Co., Inc., USA; Mills, Sander G.; Springer, Martin S.; MacCoss, Malcolm

SOURCE: PCT Int. Appl., 185 pp.

CODEN: PIXXD2

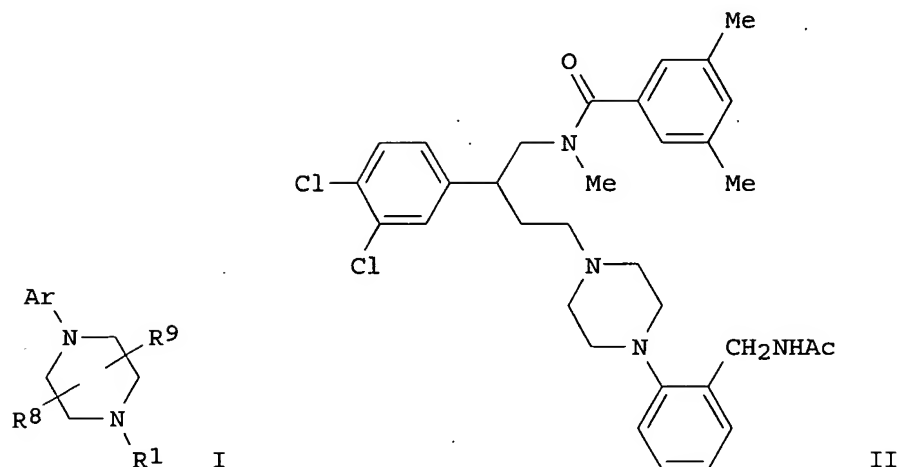
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO.  | DATE       |
|---|------|----------|------------------|------------|
| WO 9825617  | A1   | 19980618 | WO 1997-US22769  | 19971212   |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                  |            |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG  |      |          |                  |            |
| AU 9855224  | A1   | 19980703 | AU 1998-55224    | 19971212   |
| PRIORITY APPLN. INFO.:  |      |          | US 1996-32889P   | P 19961213 |
|   |      |          | US 1996-33567P   | P 19961220 |
|   |      |          | WO 1997-US22769  | W 19971212 |
| OTHER SOURCE(S):  |      |          | MARPAT 129:81753 |            |
| GI  |      |          |                  |            |



AB The title compds. [I; R<sup>1</sup> = (un)substituted C1-8 alkyl, C1-8 alkenyl; the nitrogen attached to R<sup>1</sup> is optionally quaternized with C1-4 alkyl or phenylC1-4alkyl or is optionally present as N-oxide; Ar = (un)substituted Ph, pyridyl, pyrimidyl, etc.; R<sup>8</sup>, R<sup>9</sup> = H, (un)substituted C1-4 alkyl], useful as modulators of chemokine receptor activity, were prepared. Thus, 5-step synthesis of the title compound 3(S)-II starting from 3,5-dimethylbenzoic acid and 3(S)-(3,4-dichlorophenyl)-4-methylamino-1-pentene was described. In particular, compds. I are useful as modulators of the chemokine receptors CCR-1, CCR-2, CCR-2A, CCR-2B, CCR-3, CCR-4, CCR-5, CXCR-3, and/or CXCR-4. Compds. I can be used for preventing infection by HIV, treating infection by HIV, delaying of the onset of AIDS, or treating AIDS. Compds. I are effective at 0.1-5 mg/kg/day.

IC ICM A61K031-495

ICS A61K031-50

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

IT 179249-56-0P 179249-57-1P 179249-58-2P 179249-59-3P 179249-60-6P  
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179250-11-4P 179250-12-5P 179250-13-6P **179250-57-8P**  
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209160-72-5P 209160-73-6P 209160-74-7P 209160-75-8P 209160-76-9P  
209160-77-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

IT 92-54-6, 1-Phenylpiperazine 100-07-2, p-Anisoyl chloride 109-00-2, 3-Hydroxypyridine 142-08-5, 2(1H)-Pyridinone 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 288-94-8, 1H-Tetrazole 394-47-8, o-Fluorobenzonitrile 446-52-6, 2-Fluorobenzaldehyde 499-06-9, 3,5-Dimethylbenzoic acid 725-89-3, 3,5-Bis(trifluoromethyl)benzoic acid 785-56-8, 3,5-Bis(trifluoromethyl)benzoyl chloride 1493-27-2, o-Fluoronitrobenzene 2905-62-6, 3,5-Dichlorobenzoyl chloride 13058-77-0, 8-Chloro-1,7-naphthyridine 39512-51-1, 1-(2-Methylphenyl)piperazine 52341-91-0 57260-71-6 72762-00-6, 2-Hydroxypyridine 74803-32-0 84400-99-7, 7-Chlorofuro[2,3-c]pyridine 90719-32-7, 4(S)-Benzyl-2-oxazolidinone 111896-72-1 121371-44-6 147643-57-0 156300-01-5 179250-63-6 179250-64-7 179250-65-8 179250-66-9 209160-84-9 209160-85-0 209160-86-1 209160-87-2 209160-88-3 209160-89-4 209160-90-7 209160-92-9 209160-93-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

IT 59084-06-9P 59215-38-2P 91646-29-6P 164328-62-5P 164329-19-5P 164329-21-9P 167483-86-5P 167484-59-5P 170017-73-9P 170017-74-0P 174855-53-9P 174855-57-3P 174855-59-5P 179250-25-0P 179250-27-2P 179250-28-3P 179250-29-4P 179250-30-7P 179250-31-8P 179250-32-9P 179250-33-0P 179250-34-1P 179250-35-2P 179250-36-3P 179250-37-4P 179250-38-5P 179250-39-6P 179250-40-9P 179250-41-0P 179250-42-1P 179250-43-2P 179250-44-3P 179250-45-4P 179250-46-5P 179250-47-6P 179250-48-7P 179250-49-8P 179250-50-1P 179250-51-2P 179250-52-3P 179250-53-4P 179250-54-5P 179250-55-6P 179250-56-7P 179250-58-9P 179250-59-0P 179250-60-3P 179250-61-4P 199105-20-9P 209160-78-1P 209160-79-2P 209160-80-5P 209160-81-6P 209160-82-7P 209160-91-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

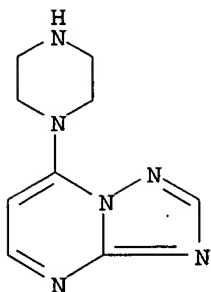
IT 179250-57-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

RN 179250-57-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



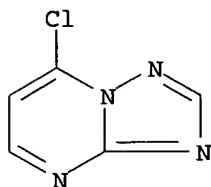
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IT 52341-91-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of substituted aryl piperazines as modulators of  
chemokine receptor activity)

RN 52341-91-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-chloro- (9CI) (CA INDEX NAME)

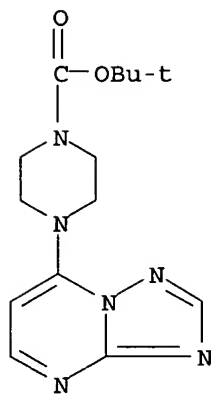


IT 179250-56-7P 179250-58-9P

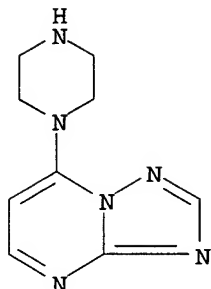
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of substituted aryl piperazines as modulators of  
chemokine receptor activity)

RN 179250-56-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl-,  
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 179250-58-9 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(1-piperazinyl)- (9CI) (CA INDEX NAME)

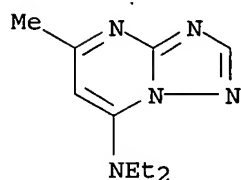


REFERENCE COUNT: 4. THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1996:306356 HCAPLUS  
 DOCUMENT NUMBER: 124:352464  
 TITLE: Modulation of the dissolution profiles from Geomatrix multi-layer matrix tablets containing drugs of different solubility  
 AUTHOR(S): Conte, U.; Maggi, L.  
 CORPORATE SOURCE: Dep. Pharmaceutical Chem., Univ. Pavia, Pavia, I-27100, Italy  
 SOURCE: Biomaterials (1996), 17(9), 889-896  
 CODEN: BIMADU; ISSN: 0142-9612  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A new multi-layer tablet design consists in the application of a drug-free barrier layer on one or both bases of an active core (hydrophilic matrix). The partial coating modulates the core hydration process and reduces the surface area available for drug release. The result is an extended release that draws close to a linear profile. The device was mainly intended for soluble drugs, while an excessive reduction of the release rate may be obtained with drugs of low solubility. In this study a new time-dependent polymeric barrier is proposed to control the release of sparingly soluble drugs. Two different barrier compns. (one swellable and one erodible) are applied on active cores containing drugs of different water solubility, trapidil, ketoprofen and nicardipine-HCl, and the drug dissoln. patterns of the different multi-layer devices are compared. During dissoln., the swellable barrier swells and gels, but is not eroded, thus acting as a modulating membrane during the release process. The erodible barrier, instead, is progressively removed by the dissoln. medium, exposing in time an increasing extent of the planar surface(s) of the core to interaction with the outer environment and to drug release. Both types of coatings are able to control drug release from the devices: the swellable barrier shows a stronger modulation efficiency and is more suitable to modify the delivery pattern of highly soluble drugs; the erodible barrier shows a time-dependent coating effect that provides better control of the dissoln. profile of sparingly soluble drugs.

CC 63-5 (Pharmaceuticals)  
 IT 15421-84-8, Trapidil 22071-15-4, Ketoprofen 54527-84-3,  
 Nicardipine hydrochloride  
 RL: PEP (Physical, engineering or chemical process); THU (Therapeutic  
 use); BIOL (Biological study); PROC (Process); USES (Uses)  
 (modulation of dissoln. profiles from Geomatrix multi-layer  
 matrix tablets)  
 IT 15421-84-8, Trapidil  
 RL: PEP (Physical, engineering or chemical process); THU (Therapeutic  
 use); BIOL (Biological study); PROC (Process); USES (Uses)  
 (modulation of dissoln. profiles from Geomatrix multi-layer  
 matrix tablets)  
 RN 15421-84-8 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA  
 INDEX NAME)



L24 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:701937 HCAPLUS

DOCUMENT NUMBER: 123:313997

TITLE: Preparation of 7-phenoxyalkyl-1,2,4-triazolo[1,5-a]pyrimidines for treatment of seizures and neurological disorders.

INVENTOR(S): Heal, David John; Fernandez, Fernandez Maria Isab;  
 Sargent, Bruce Jeremy

PATENT ASSIGNEE(S): Boots Co. PLC, UK

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

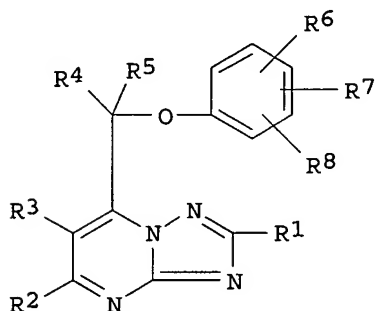
PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| WO 9510521  | A1   | 19950420 | WO 1994-EP3364  | 19941012 |
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| RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG  |      |          |                 |          |
| IN 179169   | A    | 19970906 | IN 1994-MA982   | 19941011 |
| CA 2173857  | AA   | 19950420 | CA 1994-2173857 | 19941012 |
| AU 9478554  | A1   | 19950504 | AU 1994-78554   | 19941012 |
| AU 679573   | B2   | 19970703 |                 |          |
| ZA 9407949  | A    | 19960123 | ZA 1994-7949    | 19941012 |
| EP 723546   | A1   | 19960731 | EP 1994-929537  | 19941012 |

|   |    |          |                |          |
|---|----|----------|----------------|----------|
| EP 723546   | B1 | 20000119 |                |          |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE |    |          |                |          |
| CN 1135754  | A  | 19961113 | CN 1994-194265 | 19941012 |
| CN 1040537  | B  | 19981104 |                |          |
| HU 74580  | A2 | 19970128 | HU 1996-959    | 19941012 |
| JP 09503771   | T2 | 19970415 | JP 1994-511287 | 19941012 |
| BR 9407812  | A  | 19970506 | BR 1994-7812   | 19941012 |
| IL 111259   | A1 | 19980208 | IL 1994-111259 | 19941012 |
| RU 2136684  | C1 | 19990910 | RU 1996-108927 | 19941012 |
| PL 177920   | B1 | 20000131 | PL 1994-313970 | 19941012 |
| ES 2142413  | T3 | 20000416 | ES 1994-929537 | 19941012 |
| RO 117020   | B1 | 20010928 | RO 1996-795    | 19941012 |
| SK 282329   | B6 | 20020107 | SK 1996-437    | 19941012 |
| NO 9601435  | A  | 19960610 | NO 1996-1435   | 19960411 |
| FI 9601630  | A  | 19960412 | FI 1996-1630   | 19960412 |
| US 5753665  | A  | 19980519 | US 1996-628662 | 19960625 |
| IN 182801   | A  | 19990724 | IN 1996-MA1544 | 19960904 |
| GR 3032480  | T3 | 20000531 | GR 2000-400175 | 20000126 |

PRIORITY APPLN. INFO.: GB 1993-21162 A 19931013  
IN 1994-MA982 A1 19941011  
WO 1994-EP3364 W 19941012

OTHER SOURCE(S): MARPAT 123:313997  
GI



I

AB Title compds. [I; R1 = H, (substituted) alkyl, alkoxy, alkanoyl; R2, R3 = H, (substituted) alkyl, alkoxy, alkanoyl, alkylthio, alkylsulfinyl, alkylsulfonyl; R4, R5 = H, (substituted) alkyl; R4R5C = C3-6 (substituted) cycloalkylidene; R6, R7, R8 = H, halo, OH, SH, cyano, (substituted) alkyl, alkanoyl, alkoxy, alkoxycarbonyl, CO<sub>2</sub>H, alkanoyloxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylsulfonylamino, sulfamoyl, carbamoyl, alkylcarbamoyl, alkanoylamino] were prepared. Thus, 4-fluorophenol was stirred 30 min. with NaH in 1,2-dimethoxyethane; 7-(1-bromoethyl)-1,2,4-triazolo[1,5-a]pyrimidine (preparation given) in 1,2-dimethoxyethane was added and the mixture was stirred 24 h to give 7-[1-(4-fluorophenoxy)ethyl]-1,2,4-triazolo[1,5-a]pyrimidine. II antagonized (+)-bicuculline-induced myoclonic seizures in mice with ED<sub>50</sub> = 13.9 mg/kg orally. The activity of I may arise from the ability to potentiate transmission of GABA and/or the ability to activate potassium channels in neurons.

IC ICM C07D487-04

ICS A61K031-505

ICI C07D487-04, C07D249-00, C07D239-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT 165383-11-9P 165383-12-0P 165383-13-1P

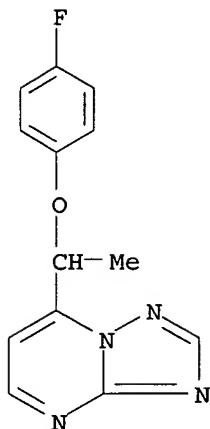
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 165383-52-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 7-phenoxyalkyl-1,2,4-triazolo[1,5-a]pyrimidines for treatment of seizures and neurol. disorders)

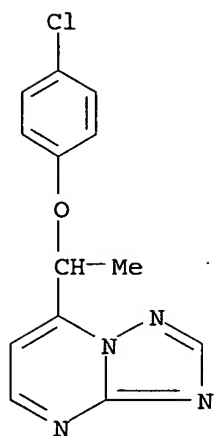
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 7-phenoxyalkyl-1,2,4-triazolo[1,5-a]pyrimidines for treatment of seizures and neurol. disorders)

RN 165383-11-9 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-fluorophenoxy)ethyl]- (9CI) (CA INDEX NAME)

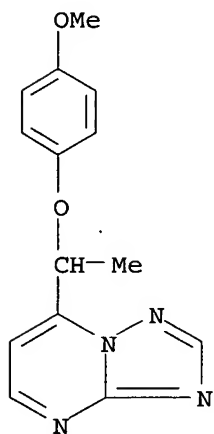


RN 165383-12-0 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-chlorophenoxy)ethyl]- (9CI) (CA INDEX NAME)



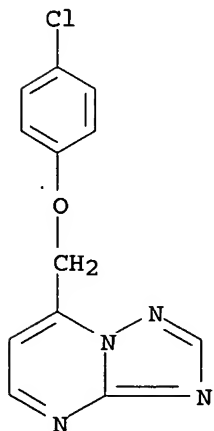
RN 165383-13-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-methoxyphenoxy)ethyl]- (9CI)  
(CA INDEX NAME)

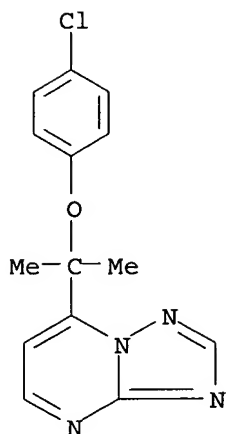


RN 165383-14-2 HCAPLUS

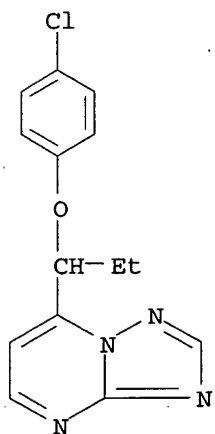
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[(4-chlorophenoxy)methyl]- (9CI) (CA  
INDEX NAME)



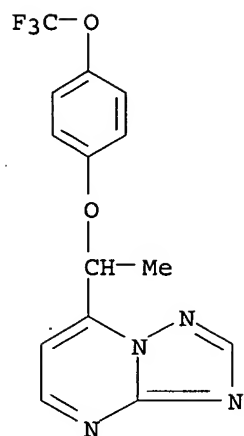
RN 165383-15-3 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-chlorophenoxy)-1-methylethyl]-  
 (9CI) (CA INDEX NAME)



RN 165383-16-4 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-chlorophenoxy)propyl]- (9CI)  
 (CA INDEX NAME)

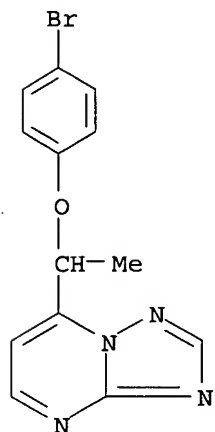


RN 165383-17-5 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(trifluoromethoxy)phenoxy]ethyl]-  
 (9CI) (CA INDEX NAME)



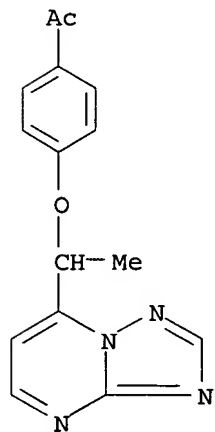
RN 165383-18-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-bromophenoxy)ethyl]- (9CI) (CA INDEX NAME)



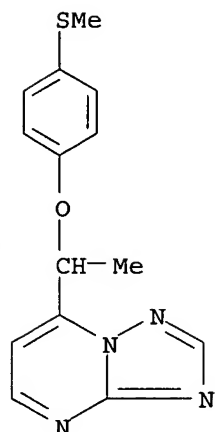
RN 165383-19-7 HCAPLUS

CN Ethanone, 1-[4-(1-[1,2,4]triazolo[1,5-a]pyrimidin-7-ylethoxy)phenyl]- (9CI) (CA INDEX NAME)



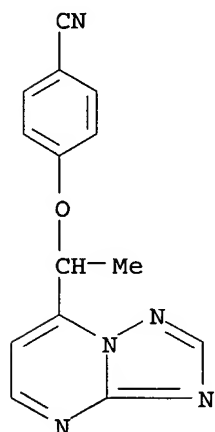
RN 165383-20-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(methylthio)phenoxy]ethyl]-(9CI) (CA INDEX NAME)



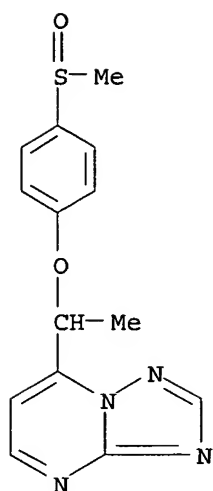
RN 165383-21-1 HCAPLUS

CN Benzonitrile, 4-(1-[1,2,4]triazolo[1,5-a]pyrimidin-7-ylethoxy)-(9CI) (CA INDEX NAME)



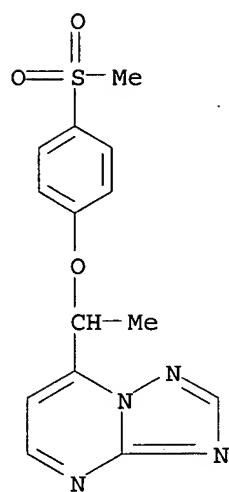
RN 165383-22-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(methylsulfinyl)phenoxy]ethyl]-(9CI) (CA INDEX NAME)



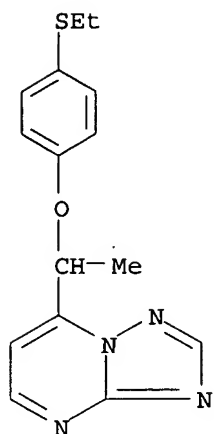
RN 165383-23-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(methylsulfonyl)phenoxy]ethyl]-  
(9CI) (CA INDEX NAME)



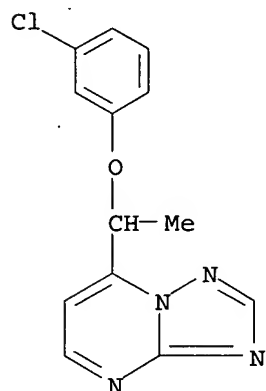
RN 165383-24-4 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(ethylthio)phenoxy]ethyl]- (9CI)  
(CA INDEX NAME)



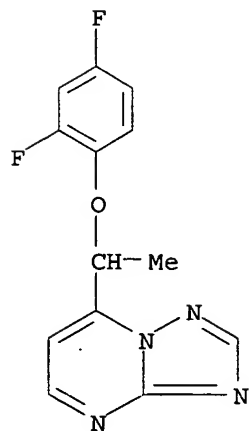
RN 165383-25-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(3-chlorophenoxy)ethyl] - (9CI) (CA INDEX NAME)



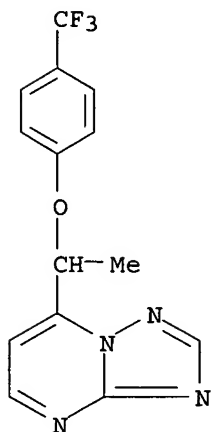
RN 165383-26-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(2,4-difluorophenoxy)ethyl] - (9CI) (CA INDEX NAME)



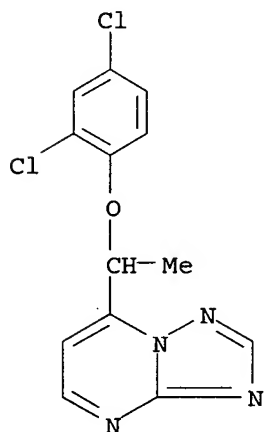
RN 165383-27-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(trifluoromethyl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)



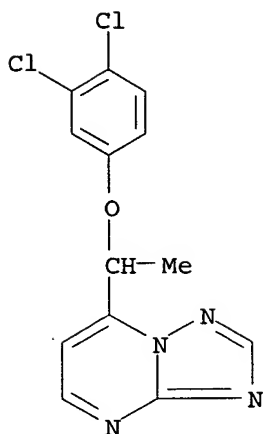
RN 165383-28-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(2,4-dichlorophenoxy)ethyl]- (9CI) (CA INDEX NAME)

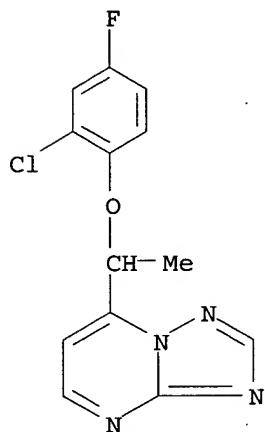


RN 165383-29-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(3,4-dichlorophenoxy)ethyl]- (9CI) (CA INDEX NAME)

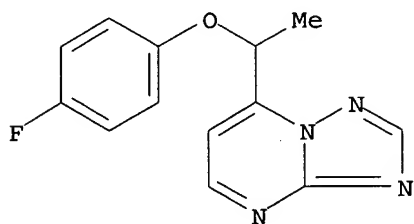


RN 165383-30-2 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(2-chloro-4-fluorophenoxy)ethyl]-  
 (9CI) (CA INDEX NAME)



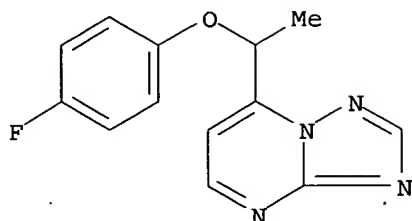
RN 165383-49-3 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-fluorophenoxy)ethyl]-, (+)-  
 (9CI) (CA INDEX NAME)

Rotation (+).



RN 165383-50-6 HCAPLUS  
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-fluorophenoxy)ethyl]-, (-)-  
 (9CI) (CA INDEX NAME)

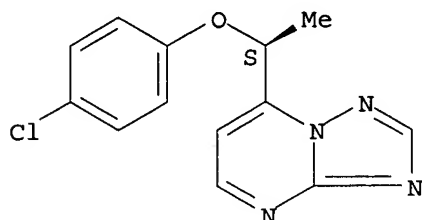
Rotation (-).



RN 165383-51-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[(1S)-1-(4-chlorophenoxy)ethyl]- (9CI)  
(CA INDEX NAME)

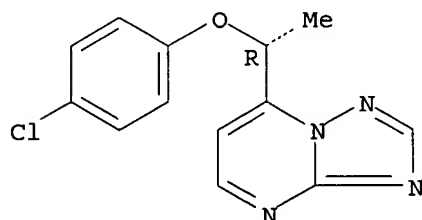
Absolute stereochemistry. Rotation (+).



RN 165383-52-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[(1R)-1-(4-chlorophenoxy)ethyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:379 HCAPLUS

DOCUMENT NUMBER: 112:379

TITLE: Effect of trapidil (Rocornal) and its derivatives on the calcium current in cultured **neurones** and the effect of the trapidil derivative AR 12456 on contraction parameters of different cardiovascular preparations

AUTHOR(S): Bodewei, Rolf; Flederwisch, I.; Hering, S.; Schubert, B.; Warbanov, W.

CORPORATE SOURCE: Bereich. Zell. Mol. Kardiol., Wiss. DDR, Berlin, DDR-1115, Ger. Dem. Rep.

SOURCE: Wissenschaftliche Zeitschrift der Ernst-Moritz-Arndt-Universitaet Greifswald, Medizinische Reihe (1988),

37(2-3), 58-66

CODEN: WZERDH; ISSN: 0138-1067

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The effects of trapidil and AR 12456 on Ca influx in cultured neuroblastoma-glioma hybrid cells and on contractility of rabbit heart and artery preps. and of neonatal rat heart cells were studied by electrophysiol methods. At relatively high concns. both agents had Ca-antagonist and neg. inotropic effects. There may be tissue-specific differences in Ca channel responses to trapidil and related compds.

CC 1-8 (Pharmacology)

ST trapidil AR 12456 calcium channel neuron; artery heart contraction trapidil AR 12456

IT 15421-84-8, Trapidil 100557-06-0, AR-12456

RL: BIOL (Biological study)

(heart and artery contractility and neuronal calcium influx response to)

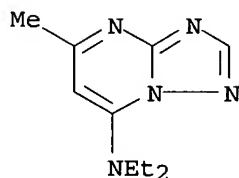
IT 15421-84-8, Trapidil

RL: BIOL (Biological study)

(heart and artery contractility and neuronal calcium influx response to)

RN 15421-84-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA INDEX NAME)



L24 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:107854. HCAPLUS

DOCUMENT NUMBER: 110:107854

TITLE: Effects of trapidil and trapidil derivatives on arachidonic acid and prostaglandin endoperoxide analog U 46619-induced blood pressure changes in rats

AUTHOR(S): Heinroth-Hoffmann, I; Hauser, A.; Taube, C.; Mest, H. J.

CORPORATE SOURCE: Dep. Pharmacol. Toxicol., Martin Luther Univ., Halle, 4020, Ger. Dem. Rep.

SOURCE: Biomedica Biochimica Acta (1989), 47(10-11), S145-S148  
CODEN: BBIADT; ISSN: 0232-766X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The influence of trapidil (T) and two 5,7-disubstituted 1,2,4-triazolo[1,5-a]pyrimidine derivs. (TD, AR 12456 and AR 12463) on blood pressure changes induced by arachidonic acid (AA) and the prostaglandin endoperoxide analog U 46619 was studied in normotensive rats in comparison with the effects of the cyclooxygenase inhibitor acetylsalicylic acid (ASA) and the TXA2 antagonist BM 13177. ASA and AR 12456 completely eliminated the second blood pressure depression after injection of AA and simultaneously diminished TXA2, TXB2 and 6-keto-PGF1 $\alpha$  formation in murine blood, whereas BM 13177 prevented

the return of the blood pressure to the preinjection level after the initial brief fall in arterial pressure. BM 13177 and AR 12463 reduced the rise in U 46619-provoked blood pressure by 75 and 58%, resp. Trapidil had no effect on blood pressure changes stimulated by AA and U 46619.

CC 1-8 (Pharmacology)

IT 15421-84-8, Trapidil 100557-04-8, AR 12463 100557-06-0, AR 12456

RL: BIOL (Biological study)

(blood pressure response to arachidonic acid and U-46619 modulation by)

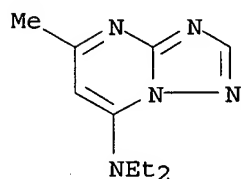
IT 15421-84-8, Trapidil

RL: BIOL (Biological study)

(blood pressure response to arachidonic acid and U-46619 modulation by)

RN 15421-84-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA INDEX NAME)



L24 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:413792 HCAPLUS

DOCUMENT NUMBER: 85:13792

TITLE: Pharmacology of trapymin. 2. Analysis of the mode of action

AUTHOR(S): Ohnishi, Haruo; Tsukuda, Shigeru; Yamaguchi, Kazuo; Ogawa, Nobuhisa; Uchiyama, Toshimitsu; Ito, Ryuta

CORPORATE SOURCE: Res. Lab. Pharmacol., Mochida Pharm. Co., Ltd., Tokyo, Japan

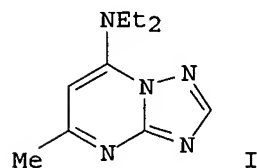
SOURCE: Nippon Yakurigaku Zasshi (1975), 71(7), 727-38

CODEN: NYKZAU; ISSN: 0015-5691

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



AB Trapymin (I) [15421-84-8] (10-5-10-4M) relaxed the isolated renal, pulmonary, femoral, and mesenteric arteries in rabbits, and coronary arteries in pigs. These relaxations were not antagonized by propranolol.

I was effective on vasopressin-induced angina in rats and electrocoagulation-induced myocardial infarction in rabbits, and suppressed adrenaline-induced arrhythmia but not  $\text{CaCl}_2$ -induced arrhythmia in rats. I reduced catechol amine content in brain, adrenals, and heart, but had no effect on monoamine oxidase in brain and liver of rats. I showed ganglion-blocking and neuron-blocking effects on cervical ganglions in cats.  $\text{Na}^+$ -,  $\text{K}^+$ -dependent ATPase of bovine heart and P/O ratio of mitochondria of rat heart were not affected by I. The action of I is papaverine [58-74-2]-like and mediated by  $\beta$ -receptors.

CC 1-5 (Pharmacodynamics)

IT 15421-84-8

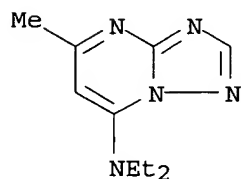
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pharmacol. of)

IT 15421-84-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pharmacol. of)

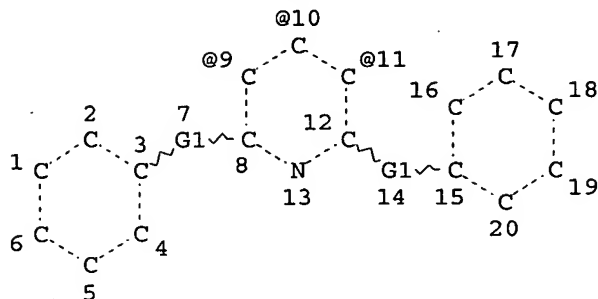
RN 15421-84-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA INDEX NAME)



=> d que  
L25

STR



S @21

S ~ O  
@22 23

G2 @24

Ak @25      O @26      S @27      N @28

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VAR G1=21/22/SO2
VAR G2=25/26/27/28/NO2/CN
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DEFAULT ECLEVEL IS LIMITED

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GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 28

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L28 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2004:41501 HCAPLUS  
DOCUMENT NUMBER: 140:87744  
TITLE: Affinity small molecules for the EPO receptor  
INVENTOR(S): Olsson, Lennart; Naranda, Tatjana  
PATENT ASSIGNEE(S): Receptron, Inc., USA  
SOURCE: PCT Int. Appl., 85 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

| PATENT NO.    | KIND   | DATE     | APPLICATION NO. | DATE     |
|---------------|--|----------|-----------------|----------|
| WO 2004005323 | A2   | 20040115 | WO 2003-US21394 | 20030703 |
| W:            | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |          |
| RW:           | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG   |          |                 |          |

PRIORITY APPLN. INFO.: US 2002-393360P P 20020703  
 US 2002-393361P P 20020703  
 US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

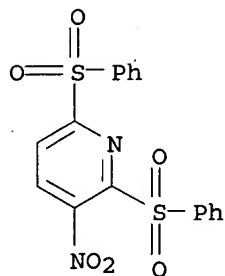
AB Comps. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject comps. in a physiol. environment. The comps. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

IT 259683-29-9

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

RN 259683-29-9 HCAPLUS

CN Pyridine, 3-nitro-2,6-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



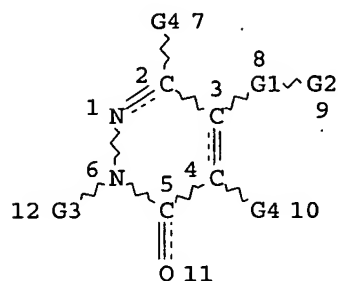
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Ward PCT/US03/21394

=> d que l32

L29

STR



S @13

S~O  
@14 15

N @16

Cb @17

Hy @18

Hy @19

Ak @20

O @21

NH^S  
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VAR G2=17/18/19

VAR G3=H/20

VAR G4=H/21/22/NO2/CN/24

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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L31 29 SEA FILE=REGISTRY SSS FUL L29

L32 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L31

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L32 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:623925 HCAPLUS

DOCUMENT NUMBER: 138:106662

TITLE: Synthesis of [1,4]benzodioxino[2,3-c and  
2,3-d]pyridazinones

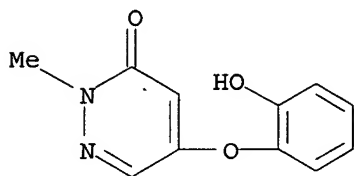
AUTHOR(S): Chung, Hyun-A.; Kim, Jeum-Jong; Cho, Su-Dong; Lee,  
Sang-Gyeong; Yoon, Yong-Jin; Kim, Sung-Kyu

CORPORATE SOURCE: Department of Chemistry and Research Institute of

Searched by Paul Schulwitz

Natural Sciences College of Natural Sciences,  
Gyeongsang National University, Jinju, 660-701, S.  
Korea

SOURCE: Journal of Heterocyclic Chemistry (2002), 39(4),  
685-689  
CODEN: JHTCAD; ISSN: 0022-152X  
PUBLISHER: HeteroCorporation  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:106662  
AB Reaction of chloropyridazin-3-ones with catechol in the presence of  
potassium carbonate gave the corresponding [1,4]benzodioxino[2,3-c and/or  
2,3-d]pyridazinones.  
IT **485808-28-4P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of benzodioxinopyridazinones via reaction of catechol with  
chloropyridazinones in presence of potassium carbonate catalyst)  
RN 485808-28-4 HCAPLUS  
CN 3(2H)-Pyridazinone, 5-(2-hydroxyphenoxy)-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:645926 HCAPLUS

DOCUMENT NUMBER: 129:302606

TITLE: Dehalogenation of 1-methyl-5-halo-4-substituted-  
pyridazin-6-ones

AUTHOR(S): Kweon, Deok-Heon; Kang, Young-Jin; Chung, Hyun-A.;  
Yoon, Yong-Jin

CORPORATE SOURCE: Department of Chemistry & Research Institute of  
Natural Sciences, Gyeongsang National University,  
Jinju, 660-701, S. Korea

SOURCE: Journal of Heterocyclic Chemistry (1998), 35(4),  
819-826

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal

LANGUAGE: English

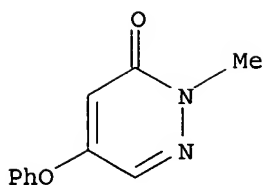
AB In order to confirm the regiochem. for the functionalization of  
1-(1,1-dibromo-2-oxopropyl)-4,5-dihalopyridazin-6-ones, the dehalogenation  
of 1-methyl-5-halo-4-substituted-pyridazin-6-ones using Pd/C and hydrogen  
was carried out. The results of the title reaction are reported.

IT **214556-22-6P 214556-23-7P**

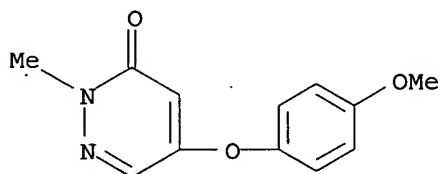
RL: SPN (Synthetic preparation); PREP (Preparation)  
(dehalogenation of halopyridazinones)

RN 214556-22-6 HCAPLUS

CN 3(2H)-Pyridazinone, 2-methyl-5-phenoxy- (9CI) (CA INDEX NAME)



RN 214556-23-7 HCAPLUS  
 CN 3 (2H)-Pyridazinone, 5-(4-methoxyphenoxy)-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:521682 HCAPLUS

DOCUMENT NUMBER: 127:214594

TITLE: Pharmacophore requirements in new series of pyridazinyl alkanolic acids, N-[(pyridazin-2-yl) alkyl] succinyl and glutaryl amides, inhibitors of thromboxane A2 biosynthesis

AUTHOR(S): Moreau, S.; Coudert, P.; Lasserre, B.; Vallee-Goyet, D.; Gardette, D.; Navarro-Delmasure, C.; Chanh, A. Pham Huu; Dossou-Gbete, V.; Couquelet, J.

CORPORATE SOURCE: Groupe de Recherches en Pharmacochimie Laboratoire de Chimie Therapeutique Faculte de Pharmacie 28, Clermont-Ferrand, F-63001, Fr.

SOURCE: Prostaglandins, Leukotrienes and Essential Fatty Acids (1997), 56(6), 431-436

CODEN: PLEAEU; ISSN: 0952-3278

PUBLISHER: Churchill Livingstone

DOCUMENT TYPE: Journal

LANGUAGE: English

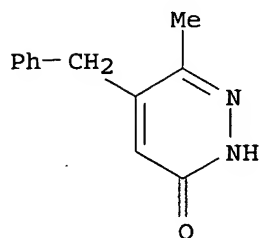
AB New series of 5-benzyl-6-methyl-4-oxo pyridazin-2-yl alkanolic acids, N-[(pyridazin-2-yl)alkyl] succinyl and glutaryl amides have been synthesized and evaluated in vitro as TXA2 biosynthesis inhibitors. The expts. were carried out using arachidonic acid (32.8  $\mu$ M) as a substrate and horse platelet microsomes as sources of TXA2 synthase. The presence of TXB2, a stable metabolite of TXA2, was determined by RIA. The potency of active compds. ( $1.10^{-4} < IC_{50} < 1.10^{-6}$  M) greatly depends on the length of the chain at the N-2 position on the pyridazine ring. Furthermore, enzyme inhibition in vitro is increased with the presence of a halogen atom on the aromatic moiety of the benzyl group at C-5. The compound having a pentanoic side chain and a 4-fluoro benzyl moiety was the most active derivative with an  $IC_{50}$  value of  $6.69 \times 10^{-6}$  M. Mol. modeling studies were done on all the synthesized pyridazinones and on prostaglandin H2 (PGH2) suggesting spatial features and vols. of TXA2 synthase pharmacophore mode in these series of derivs.

IT 173429-17-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant; pharmacophore requirements in a new series of pyridazinyl  
 alkanolic acids as inhibitors of thromboxane A2 biosynthesis)

RN 173429-17-9 HCAPLUS

CN 3(2H)-Pyridazinone, 6-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



L32 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:623003 HCAPLUS

DOCUMENT NUMBER: 125:238690

TITLE: Ligands for the SH2 domain of the src protein for  
 treatment of bone resorption diseases

INVENTOR(S): Dunnington, Damien John

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: Eur. Pat. Appl., 46 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| EP 727211   | A1   | 19960821 | EP 1996-200270  | 19960207 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE   |      |          |                 |          |
| AU 9644404  | A1   | 19960822 | AU 1996-44404   | 19960207 |
| ZA 9601000  | A    | 19960807 | ZA 1996-1000    | 19960208 |
| CA 2169136  | AA   | 19960811 | CA 1996-2169136 | 19960208 |
| ZA 9601001  | A    | 19960813 | ZA 1996-1001    | 19960208 |
| CN 1135333  | A    | 19961113 | CN 1996-104364  | 19960208 |
| CN 1137378  | A    | 19961211 | CN 1996-105740  | 19960208 |
| JP 09087200   | A2   | 19970331 | JP 1996-59921   | 19960208 |
| CA 2212645  | AA   | 19960815 | CA 1996-2212645 | 19960209 |
| WO 9624343  | A1   | 19960815 | WO 1996-US1964  | 19960209 |
| W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN |      |          |                 |          |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG  |      |          |                 |          |
| AU 9649237  | A1   | 19960827 | AU 1996-49237   | 19960209 |
| EP 809490   | A1   | 19971203 | EP 1996-905494  | 19960209 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI   |      |          |                 |          |
| BR 9607614  | A    | 19980609 | BR 1996-7614    | 19960209 |
| JP 10513474   | T2   | 19981222 | JP 1996-524486  | 19960209 |
| WO 9624847  | A1   | 19960815 | WO 1996-US2490  | 19960212 |

W: JP, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

EP 811159 A1 19971210 EP 1996-906615 19960212

R: BE, CH, DE, DK, FR, GB, IT, LI, NL

JP 10513564 T2 19981222 JP 1996-524493 19960212

ZA 9601318 A 19970127 ZA 1996-1318 19960220

ZA 9605499 A 19980330 ZA 1996-5499 19960628

ZA 9605500 A 19980330 ZA 1996-5500 19960628

FI 9703259 A 19971008 FI 1997-3259 19970807

NO 9703659 A 19971008 NO 1997-3659 19970808

PRIORITY APPLN. INFO.:

US 1995-386381 A 19950210

US 1995-400220 A 19950307

US 1995-497357 A 19950630

US 1995-541080 A 19951011

US 1995-580868 19951229

WO 1996-US1964 W 19960209

WO 1996-US2490 W 19960212

AB A method of treating a bone resorption disease by administering a compound that binds to the SH2 domain of the human src, e.g. I, protein with a binding affinity greater than 50-fold higher than for the SH2 domains of the human lck, fyn, hcp, Grb2, SH-PTP2, and p85 is described. The preparation of a number of compds. is described. An assay system for binding of these ligands to SH2 domains using SH2 domains manufactured as fusion proteins in Escherichia coli is described. I inhibited inhibited 45Ca in a mouse embryonic ulna model with an IC50 of 19  $\mu$ M.

IT 182198-18-1P

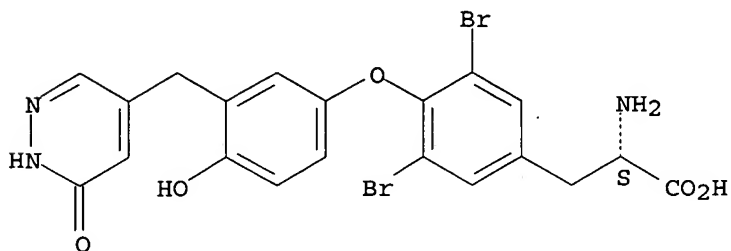
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as ligand for SH2 domain of src protein; ligands for SH2 domain of src protein for treatment of bone resorption diseases)

RN 182198-18-1 HCAPLUS

CN L-Tyrosine, 3,5-dibromo-O-[3-[(1,6-dihydro-6-oxo-4-pyridazinyl)methyl]-4-hydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:871851 HCAPLUS

DOCUMENT NUMBER: 124:86262

TITLE: Heterocyclic tautomerism. IX. Structural revision of a series of pharmacologically active pyridazines

AUTHOR(S): Guard, James A. M.; Steel, Peter J.

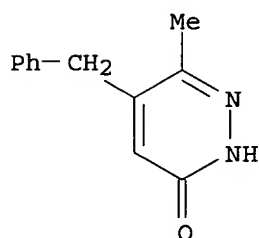
CORPORATE SOURCE: Chemistry Dep., Univ. Canterbury, Christchurch, N. Z.

SOURCE: Australian Journal of Chemistry (1995), 48(9), 1601-7

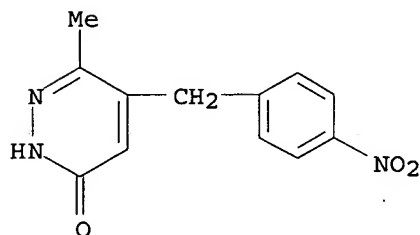
CODEN: AJCHAS; ISSN: 0004-9425

PUBLISHER: Commonwealth Scientific and Industrial Research Organization

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB On the basis of  $^1\text{H}$  NMR n.O.e. measurements and an x-ray crystal structure determination, it is shown that a large series of pharmacol. active pyridazine derivs. should be represented as aromatic pyridazine tautomers [e.g. (1b)-(3b)], rather than the previously reported arylidene-4,5-dihydropyridazines [e.g. (1a)-(3a)]. Crystals of (7b) are monoclinic,  $P2_1/c$ ,  $a$  13.312(3),  $b$  7.269(1),  $c$  11.753(2) Å,  $\beta$  101.38(3)°,  $Z = 4$ ; the structure was refined to a conventional  $R[I > 2\sigma(I)]$  0.037.  
 IT 173429-17-9  
 RL: PRP (Properties)  
 (structural revision of pharmacol. active pyridazines as tautomers)  
 RN 173429-17-9 HCAPLUS  
 CN 3(2H)-Pyridazinone, 6-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 172606-32-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (structural revision of pharmacol. active pyridazines as tautomers)  
 RN 172606-32-5 HCAPLUS  
 CN 3(2H)-Pyridazinone, 6-methyl-5-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1995:840619 HCAPLUS  
 DOCUMENT NUMBER: 123:271334  
 TITLE: 5-(2-Chlorobenzyl)-6-methyl-3(2H)-pyridazinone  
 AUTHOR(S): Moreau, Stephane; Metin, Jacques; Coudert, Pascal; Couquelet, Jacques  
 CORPORATE SOURCE: Groupe Recherche Pharmacochimie, Lab. Chimie  
 Therapeutique, Clermont-Ferrand, 63001, Fr.  
 SOURCE: Acta Crystallographica, Section C: Crystal Structure  
 Communications (1995), C51(9), 1834-6  
 CODEN: ACSCEE; ISSN: 0108-2701

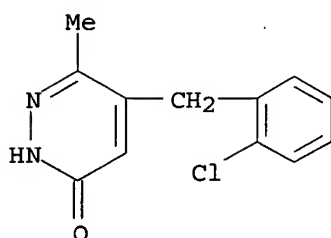
PUBLISHER: Munksgaard  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The title compound is monoclinic, space group P2<sub>1</sub>, with a 7.270(1), b 7.076(4), c 11.227(1) Å, and  $\beta$  100.57(1)°; Z = 2, dc = 1.373, dm = 1.2; R = 0.051, Rw = 0.054 for 1468 reflections. Atomic coordinates are given. The two planar rings (pyridazine and phenyl) are at an angle of .apprx.95°. Crystal cohesion is ensured by a dense network of van der Waals contacts.

IT 169136-07-6, 5-(2-Chlorobenzyl)-6-methyl-3(2H)-pyridazinone  
RL: PRP (Properties)  
(crystal structure of)

RN 169136-07-6 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-chlorophenyl)methyl]-6-methyl- (9CI) (CA INDEX NAME)



L32 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:534057 HCAPLUS

DOCUMENT NUMBER: 121:134057

TITLE: Studies on pyridazinone derivatives. XVI.  
Analgesic-antiinflammatory activities of  
3(2H)-pyridazinone derivatives

AUTHOR(S): Takaya, Masahiro; Sato, Makoto

CORPORATE SOURCE: Hamari Chem. Co., Ltd., Osaka, 533, Japan

SOURCE: Yakugaku Zasshi (1994), 114(2), 94-110

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB In order to examine analgesic and antiinflammatory activities of the position isomers of 4-ethoxy-2-methyl-5-morpholino-3(2H)-pyridazinone (emorfazone), an analgesic-antiinflammatory drug, 5-ethoxy-2-methyl-4-morpholino-3(2H)-pyridazinone, 6-ethoxy-2-methyl-4-morpholino-3(2H)-pyridazinone and 6-ethoxy-2-methyl-5-morpholino-3(2H)-pyridazinone (I) were prepared. Since I showed the most strong activity among the compds. tested, various 6-alkoxy- or 6-allyloxy-2-alkyl- or 2-cyclohexyl- or 2-phenyl-5-substituted amino-3(2H)-pyridazinones were prepared and examined for their activities. As a result, I and 2-methyl-5-morpholino-6-n-propoxy- or 6-n-butoxy-3(2H)-pyridazinone and 6-ethoxy-2-ethyl-5-morpholino-3(2H)-pyridazinone were revealed to be more potent in analgesic and antipyretic activities than com. drugs (emorfazone, aminopyrine, mepirizole, tiaramide HCl, phenylbutazone, mefenamic acid). On the basis of the available data, the structure-activity relationship in a series of 6-alkoxy-2-alkyl-5-substituted amino-3(2H)-pyridazinones was also discussed.

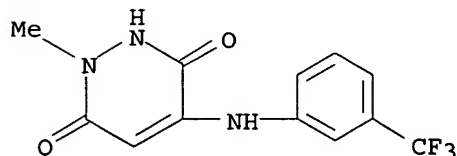
IT 88804-54-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)  
(preparation and alkylation of)

RN 88804-54-0 HCAPLUS

CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:38946 HCAPLUS

DOCUMENT NUMBER: 110:38946

TITLE: Studies on pyridazinone derivatives. XIII. Unusual displacement reaction of 5-(o-aminophenylthio)-4-chloro-2-methyl-3(2H)-pyridazinone with alkali

AUTHOR(S): Takaya, Masahiro

CORPORATE SOURCE: Hamari Chem. Co., Ltd., Osaka, 533, Japan

SOURCE: Yakugaku Zasshi (1988), 108(2), 136-41

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 110:38946

AB In order to explore the scope of an unusual displacement reaction to form 3-phenyl-10H-benzo[b]pyridazino[4,5-e][1,4]thiazine-4(3H)-one in the reaction of 5-(o-aminophenylthio)-4-chloro-2-phenyl-3(2H)-pyridazinone with NaOEt, the behavior of 2-Me (I) or 2-hydropyridazone derivs. (II) against NaOEt or NaOH were examined. Among them, I underwent an unusual displacement reaction to afford 3-methylthiazine derivative (III), 4-(o-aminophenylthio)-5-ethoxy-2-methyl-3(2H)-pyridazinone or 4-(o-aminophenylthio)-5-hydroxy-2-methyl-3(2H)-pyridazinone, but II did not.

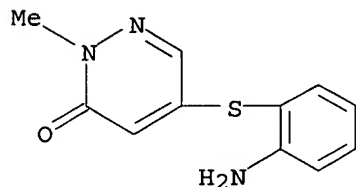
IT 118327-46-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclization-rearrangement of)

RN 118327-46-1 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-2-methyl- (9CI) (CA INDEX NAME)



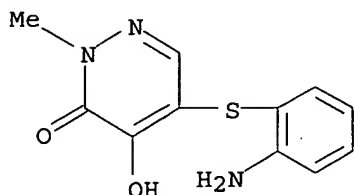
IT 51834-53-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and thermolysis of)

RN 51834-53-8 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-4-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

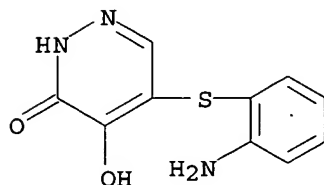


IT 118327-49-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with aqueous sodium hydroxide and thermolysis of)

RN 118327-49-4 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-4-hydroxy- (9CI) (CA INDEX NAME)



L32 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:528933 HCAPLUS

DOCUMENT NUMBER: 109:128933

TITLE: Synthesis of monochloromaleic hydrazide derivatives.  
2. Substitution of methanethiol for chlorine

AUTHOR(S): Tonegawa, Masami; Nishimura, Yukihiro; Fukasawa, Chiyoko; Kitahara, Keiichi; Yamashita, Junzo; Sato, Hisao

CORPORATE SOURCE: Tokyo Med. Coll., Tokyo, Japan

SOURCE: Tokyo Ika Daigaku Kiyo (1988), 14, 1-11

CODEN: TIDKD9; ISSN: 0385-1303

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

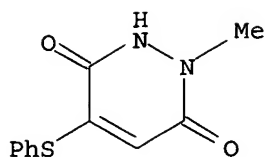
AB Substitution reactions of the title hydrazides I (R = Cl; R1 = Me, R2 = H, Me) and II (R = Cl; R1 = Me, R2 = H, Me; R1 = H, R2 = Me) with MeSNa gave the corresponding chlorine substitution products I and II (R = SMe), resp. In contrast, substitution of 4-chloro derivative I (R = Cl, R1 = H, R2 = Me) (III) with MeSNa or EtSNa gave a 1:1 mixture of 4- and 5-substituted derivs I and II (R = SMe, SEt, R1 = H, R2 = Me). Substitution of III with PhSNa gave only 4-substituted derivative I (R = SPh, R1 = H, R2 = Me).

IT 98045-61-5P

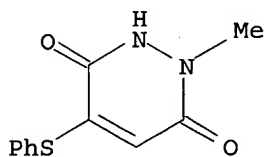
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 98045-61-5 HCAPLUS

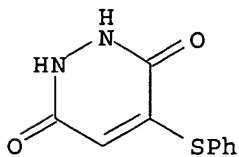
CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-(phenylthio)- (9CI) (CA INDEX NAME)



L32 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1985:504905 HCAPLUS  
 DOCUMENT NUMBER: 103:104905  
 TITLE: Synthesis of monochloromaleic hydrazide derivatives.  
 Synthesis of methylthio- and phenylthiomaleic  
 hydrazides and their N-methyl and O-acyl derivatives  
 AUTHOR(S): Satoh, Hisao; Tonegawa, Masami; Inoue, Reiko  
 CORPORATE SOURCE: Dep. Chem., Tokyo Med. Coll., Tokyo, Japan  
 SOURCE: Tokyo Ika Daigaku Kiyo (1985), 11, 1-12  
 CODEN: TIDKD9; ISSN: 0385-1303  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 AB Reaction of chloromaleic hydrazide (I; R = 4-, 5-Cl; R1 = H) with MeSH or  
 PhSH gave I (R = 4-, 5-MeS, -PhS; R1 = H), which were treated with Me2SO4  
 to give N-Me derivs. (I; R = 4-, 5-MeS, -PhS; R1 = Me). Reaction of I (R  
 = Cl, MeS, PhS; R1 = H) with PhCOCl/pyridine or Ac2O gave the  
 corresponding benzoates or acetates (II; R2 = Ph, Me).  
 IT **98045-61-5P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and acylation of)  
 RN 98045-61-5 HCAPLUS  
 CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-(phenylthio)- (9CI) (CA INDEX  
 NAME)



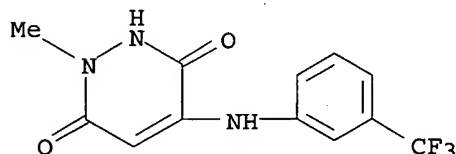
IT **98045-58-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, methylation and acylation of)  
 RN 98045-58-0 HCAPLUS  
 CN 3,6-Pyridazinedione, 1,2-dihydro-4-(phenylthio)- (9CI) (CA INDEX NAME)



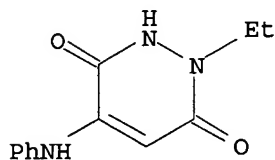
L32 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1984:85712 HCAPLUS  
 DOCUMENT NUMBER: 100:85712  
 TITLE: Pyridazines  
 PATENT ASSIGNEE(S): Morishita Pharmaceutical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|-------------|------|----------|-----------------|----------|
| JP 58183675 | A2   | 19831026 | JP 1982-66742   | 19820420 |

PRIORITY APPLN. INFO.: JP 1982-66742 19820420  
 OTHER SOURCE(S): CASREACT 100:85712  
 AB The title compds. I [R = HO, alkoxy; R1 = alkyl; R2 = H, (halo) alkyl] were prepared by reaction of I (R = halo) with the appropriate Na or K hydroxides or alkoxides. Thus, refluxing a mixture of 2.4 g I (R = Cl, R1 = Me, R2 = H), 0.46 g Na, and 50 mL EtOH for 24 h gave 1.5 g I (R = EtO, R1 = Me, R2 = H).  
 IT 88804-54-0P 88804-56-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 88804-54-0 HCAPLUS  
 CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)



RN 88804-56-2 HCAPLUS  
 CN 3,6-Pyridazinedione, 1-ethyl-1,2-dihydro-4-(phenylamino)- (9CI) (CA INDEX NAME)



L32 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1974:95822 HCAPLUS  
 DOCUMENT NUMBER: 80:95822  
 TITLE: Ring contraction of pyridazinones to pyrazols. VII  
 AUTHOR(S): Maki, Yoshifumi; Suzuki, Mikio; Takaya, Masahiro  
 CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1974), 22(1),

229-32

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

Journal

LANGUAGE:

English

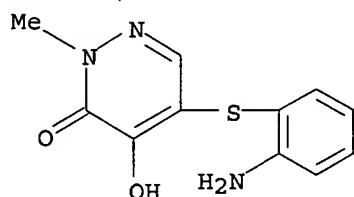
AB Previous results from the title ring contraction were extended to I. A suspension of I in 10% NaOH is heated several hr to yield II which on treatment with SOCl<sub>2</sub> in CHCl<sub>3</sub> is cyclized to III. An N<sub>2</sub>-phenyl is necessary for this type of ring contraction.

IT 51834-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 51834-53-8 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-4-hydroxy-2-methyl- (9CI) (CA  
INDEX NAME)



L32 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:456319 HCAPLUS

DOCUMENT NUMBER: 57:56319

ORIGINAL REFERENCE NO.: 57:11212b-i

TITLE: 1-Carbalkoxy-4-(aminoalkanol)piperazines

INVENTOR(S): Geschickter, Charles F.; Pierce, John S.; Chen, Ying  
H.; Reid, Ebenezer E.

SOURCE: 5 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

| PATENT NO. | KIND | DATE     | APPLICATION NO. | DATE     |
|------------|------|----------|-----------------|----------|
| US 301557  |      | 19620102 | US              | 19590528 |

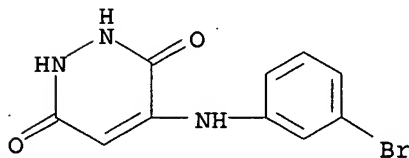
AB The title compds. (Ia) were prepared for use as inter-mediate in chemical syntheses. The Ia also had antitussive activity. A mixture of 0.05 mole 3-dibutylamino-1,2-epoxy-propane, 0.05 mole 1-carbopropoxypiperazine (I), and 50 ml. EtOH was allowed to stand 1 week, heated at 75° 8 hrs., and distilled to give 61% 1-carbopropoxy-4-(3-dibutylamino-2-hydroxy)piperazine, b0.12 162-4°. Allowing 0.029 mole I, 0.0:9 mole epichlorohydrin, and 10 ml. EtOH to stand 14 hrs., adding NaOH, Me<sub>2</sub>NH, and NaOH again (allowing the mixture to stand after each addition), and extracting with Et<sub>2</sub>O gave 75% 1-carbopropoxy-4-(3-dimethylamino-2-hydroxypropyl)-piperazine, b0.4 144-6°. Also adding 1.8 g. Me chloroformate to 6.0 g. 1-(3-dibutylamino-2-hydroxy)-trans-2,5-dimethylpiperazine, 1 ml. Et<sub>3</sub>N, and 60 ml. EtOH at 0°, adding NaOH, and extracting with Et<sub>2</sub>O gave 30% 1-carbomethoxy-4-(3-dibutylamino-2-hydroxypropyl)-trans-2,5-dimethylpiperazine, b0.25 150-3°. By one or more of the above procedures the following Ia were prepared (n, B, R, and b.p./mm, given): 0, Et<sub>2</sub>N, Me, 152-5°/0.4; 0, Et<sub>2</sub>N, Et, 138-40°/0.2; 0, Et<sub>2</sub>N, Pr, 155-7°/0.3; 0, Et<sub>2</sub>N, Bu, 172-8°/0.4; 0, Bu<sub>2</sub>N, Et, 175-9°/0.3; 0, Bu<sub>2</sub>N, Pr,

162-4°/0.12; 0, Bu2N, Bu, 176-8°/0.2; 0, morpholino, Me,  
 168-70°/0.45; 0, morpholino, Et, 205-11°/0.5; 0, morpholino,  
 Bu, 200-5°/0.6; 0, pyrrolidino, Me, 164-7°/0.7; 0,  
 pyrrolidino, Pr, 165-7°/ 0.25; 0, pyrrolidino, Bu,  
 173-5°/0.7; 0, piperidino, Et, 173-7°/0.25; 0,  
 2-methylpiperidino, Et, 184-6°/0.80; 0, 4-methylpiperidino, Me,  
 168-71°/0.4; 0, 4-methylpiperidino, Et, 173-5°/0.35; 1,  
 Me2N, Et, 192-3°/9.0; 1, Me2N, Pr, 148-50°/0.6; 1, Et2N, Et,  
 162-5°/0.6; 1, Et2N, Bu, 180-5°/0.5; 1, Bu2N, Et,  
 185-8°/0.3; 1, Bu2N, Pr, 200-2°/ 0.5; 1, Bu2N, Bu,  
 181-2°/0.15; 1, morpholino, Me, 168-70°/0.25; 1, morpholino,  
 Et, 210°/0.3; 1, morpholino, Bu, 197-8°/0.5; 1, pyrrolidino,  
 Pr, 175-8°/0.45; 1, piperidino, Et, 174-83°/0.45; 1,  
 piperidino, Pr, 187-9°/0.45; 1, 2-methylpiperidino, Bu,  
 184-6°/0.3; 1, 3-methylpiperidino, Me, 175-8°/0.4; 1,  
 4-methylpiperidino, Et, 178-80°/0.45; 2, Et2N, Bu,  
 180-4°/0.5; 2, Et2N, Et, 161-6°/0-5; 2, Me2N, Bu,  
 145-8°/0.5; 2, Et2N, Me, 155-7°/0.45; 2, Pr2N, Me,  
 155-60°/0.25; 2, Pr2N, Et, 165-7°/0-35; 2, iso-Pr2N, Et,  
 185-7°/0.45; 2, Bu2N, Me, 245-8°/8.0; 2, Bu2N, Et;  
 173-5°/0.1; 2, Bu2N, Et, 188-90°/0-5; 2, Bu2N, Pr,  
 168-70°/0.18; 2, Bu2N, Bu, 195-7°/0.1; 2, Bu2N, Bu,  
 188-91°/0.35; 2, EtBuN, Bu, 176-8°/0.3; 2, morpholino, Me,  
 175-7°/0.25; 2, morpholino, Et, 165-8°/ 0.25; 2,  
 morpholino, Pr, 169-71°/0.15; 2, morpholino, Bu,  
 210-12°/0.5; 2, pyrrolidino, Me 163-5°/0.35; 2, pyrrolidino,  
 Et, 162-3°/0.45; 2, pyrrolidino, Pr, 180-2°/0.8; 2,  
 piperidino, Et, 193°/0.2; 2, 2-methylpiperidino, Me,  
 174-6°/0.30; 2, 2-methylpiperidino Et, 175-7°/0.45; 2,  
 2-methylpiperidino Pr, 178-80°/0.3; 2, 2-methylpiperidino, Bu,  
 182-5°/0.45; 2, 3-methylpiperidino, Me, 173-5°/0.45; 2,  
 3-methylpiperidino, Et, 168-70°/0.25; 2, 4-methyl-piperidino, Bu,  
 190-2°/0.3; 4, Me2N, Me, 145-7°/0.4; 4, Et2N, Me,  
 163-5°/0.3; 4, Et2N, Et, 166-8°/0-35; 4, Bu2N, Me,  
 179-5°/0.4; 4, morpholino, Me, 179-80°/0.5; 4, morpholino,  
 Pr, 183-5°/0.4; 4, morpholino, Bu, 192-3°/0.45; 4  
 pyrrolidino, Pr, 168-70°/0.35; 4, piperidino, Me,  
 170-2°/0.45; 4, piperidino, Pr, 186-8°/0.5; 4,  
 3-methylpiperidino, Bu, 182-5°/0.4; 4, 4-methylpiperidino, Et,  
 180-2°/ 0.35; 4, 4-methylpiperidino, Bu, 190-4°/0.4.

IT 91211-30-2, 3,6-Pyridazinediol, 4-(m-bromoanilino)-  
 (preparation of)

RN 91211-30-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-bromoanilino)- (7CI) (CA INDEX NAME)



L32 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1962:456318 HCAPLUS  
 DOCUMENT NUMBER: 57:56318  
 ORIGINAL REFERENCE NO.: 57:11211h-i,11212a-b

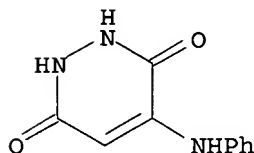
TITLE: N-(Dihydroxypyridazinyl)aniline and derivatives thereof  
 INVENTOR(S): Lowrie, Harman S.  
 PATENT ASSIGNEE(S): G.D. Searle and Co.  
 SOURCE: 2 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE     | APPLICATION NO. | DATE     |
|------------|------|----------|-----------------|----------|
| US 3037022 |      | 19620529 | US              | 19600907 |

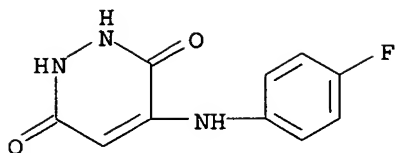
AB Compds. I are prepared by condensation of 4-chloro-3,6-dihydroxypyridazine (II) with the appropriately substituted aniline in the presence of Cu powder. Thus. a mixture of II 100, aniline 500, and Cu powder 1 part was rapidly heated to reflux. Refluxing was maintained for 25 min., the reaction mixture cooled to room temperature, and diluted with an equal volume of Et<sub>2</sub>O.

The mixture was then extracted several times with dilute KOH, the exts. back-extracted with Et<sub>2</sub>O, and then acidified with concentrated HCl. The solid, washed with H<sub>2</sub>O, and recrystd. from MeOH, gave I (Z = H), m. 262-4° (decomposition). In the same manner were prepared the following I (Z given): 4-Me (m. 247-9° decomposition), 4-Et, 4-MeO [m. 225-30° (decomposition)], 4-EtO, 4-F [m. 272-4° (decomposition)], 4-Cl [m. 276-8° (decomposition)], 4-Br, 3-Me, 3-Et, 3-MeO, 3-EtO, 3-F, 3-Cl (m. 259-62°), and 3-Br. The I bare appetite-inhibiting and diuretic activity.

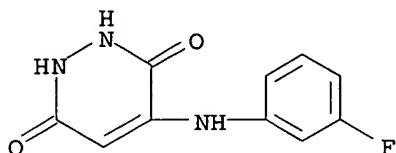
IT 90946-28-4, 3,6-Pyridazinediol, 4-anilino- (and derivs.)  
 RN 90946-28-4 HCAPLUS  
 CN 3,6-Pyridazinediol, 4-anilino- (7CI) (CA INDEX NAME)



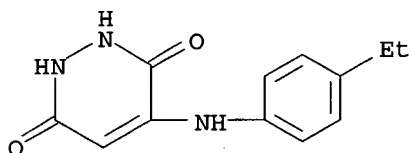
IT 782-69-4, 3,6-Pyridazinediol, 4-(p-fluoroanilino)-  
 886-25-9, 3,6-Pyridazinediol, 4-(m-fluoroanilino)-  
 88614-39-5, 3,6-Pyridazinediol, 4-(p-ethylanilino)-  
 88617-78-1, 3,6-Pyridazinediol, 4-m-phenetidino-  
 88617-79-2, 3,6-Pyridazinediol, 4-p-phenetidino-  
 89126-21-6, 3,6-Pyridazinediol, 4-(m-ethylanilino)-  
 90766-60-2, 3,6-Pyridazinediol, 4-(p-bromoanilino)-  
 90799-86-3, 3,6-Pyridazinediol, 4-(p-chloroanilino)-  
 91211-30-2, 3,6-Pyridazinediol, 4-(m-bromoanilino)-  
 91587-72-3, 3,6-Pyridazinediol, 4-(m-chloroanilino)-  
 92289-82-2, 3,6-Pyridazinediol, 4-p-toluidino- 92290-20-5  
 , 3,6-Pyridazinediol, 4-p-anisidino- 93534-86-2,  
 3,6-Pyridazinediol, 4-m-toluidino- 93534-91-9,  
 3,6-Pyridazinediol, 4-m-anisidino-  
 (preparation of)  
 RN 782-69-4 HCAPLUS  
 CN 3,6-Pyridazinediol, 4-(p-fluoroanilino)- (7CI, 8CI) (CA INDEX NAME)



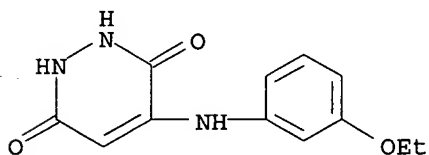
RN 886-25-9 HCAPLUS  
CN 3,6-Pyridazinediol, 4-(m-fluoroanilino)- (7CI, 8CI) (CA INDEX NAME)



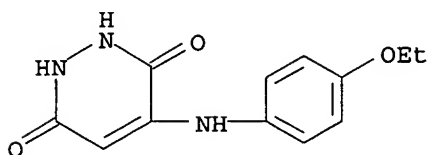
RN 88614-39-5 HCAPLUS  
CN 3,6-Pyridazinediol, 4-(p-ethylanilino)- (7CI) (CA INDEX NAME)



RN 88617-78-1 HCAPLUS  
CN 3,6-Pyridazinediol, 4-m-phenetidino- (7CI) (CA INDEX NAME)

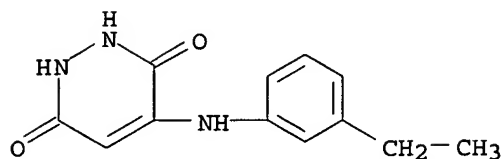


RN 88617-79-2 HCAPLUS  
CN 3,6-Pyridazinediol, 4-p-phenetidino- (7CI) (CA INDEX NAME)



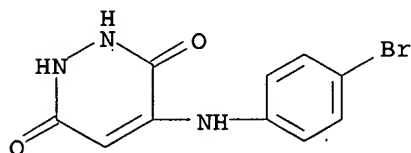
RN 89126-21-6 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-ethylanilino)- (7CI) (CA INDEX NAME)



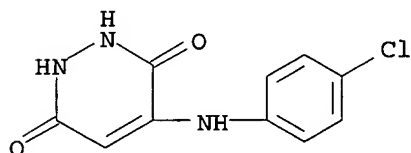
RN 90766-60-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-(p-bromoanilino)- (7CI) (CA INDEX NAME)



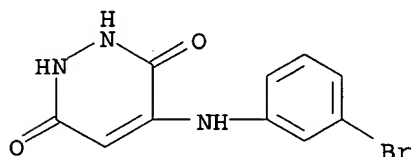
RN 90799-86-3 HCAPLUS

CN 3,6-Pyridazinediol, 4-(p-chloroanilino)- (7CI) (CA INDEX NAME)



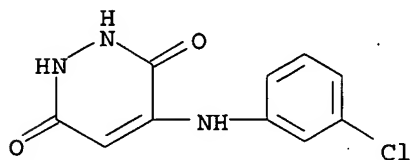
RN 91211-30-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-bromoanilino)- (7CI) (CA INDEX NAME)



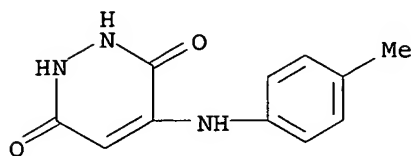
RN 91587-72-3 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-chloroanilino)- (7CI) (CA INDEX NAME)



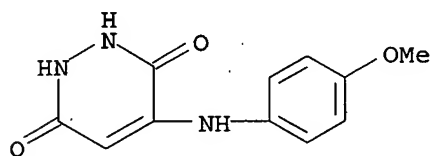
RN 92289-82-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-p-toluidino- (7CI) (CA INDEX NAME)



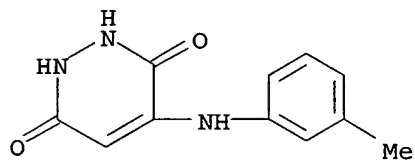
RN 92290-20-5 HCAPLUS

CN 3,6-Pyridazinediol, 4-p-anisidino- (7CI) (CA INDEX NAME)



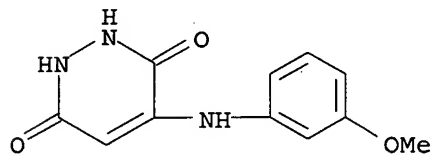
RN 93534-86-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-m-toluidino- (7CI) (CA INDEX NAME)



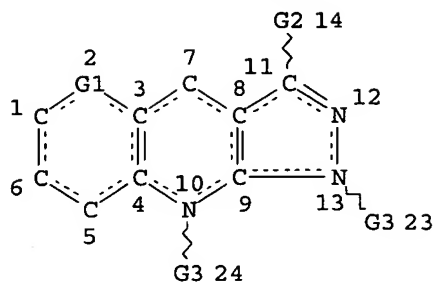
RN 93534-91-9 HCAPLUS

CN 3,6-Pyridazinediol, 4-m-anisidino- (7CI) (CA INDEX NAME)



L33

STR



C~Ak  
@15 16

C=O  
@17 18

C=S  
@19 20

C @25

C=N  
@21 22

VAR G1=CH2/15/17/19/21

VAR G2=H/25

VAR G3=H/C

NODE ATTRIBUTES:

NSPEC IS RC AT 25

CONNECT IS E3 RC AT 15

CONNECT IS E1 RC AT 16

CONNECT IS E1 RC AT 20

CONNECT IS E1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X3 C AT 16

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L35 52 SEA FILE=REGISTRY SSS FUL L33

L36 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L35

=> d l36 ibib ab hitstr 1-8

L36 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:41501 HCAPLUS

DOCUMENT NUMBER: 140:87744

TITLE: Affinity small molecules for the EPO receptor

INVENTOR(S): Olsson, Lennart; Naranda, Tatjana

PATENT ASSIGNEE(S): Receptron, Inc., USA

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------|------|----------|-----------------|----------|
| WO 2004005323 | A2   | 20040115 | WO 2003-US21394 | 20030703 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-393360P P 20020703  
US 2002-393361P P 20020703  
US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

AB Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

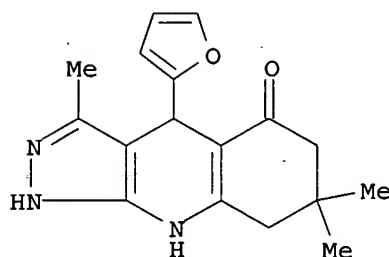
IT 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

RN 645337-25-3 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-(2-furanyl)-1,4,6,7,8,9-hexahydro-3,7,7-trimethyl- (9CI) (CA INDEX NAME)



L36 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:826097 HCAPLUS

DOCUMENT NUMBER: 136:61813

TITLE: 4-(4-Chlorophenyl)-3,7,7-trimethyl-1-[2-(4-nitrobenzoyl)ethyl]-4,7,8,9-tetrahydro-1H-pyrazolo[3,4-b]quinolin-5(6H)-one-ethanol (1/1)

AUTHOR(S): Low, John Nicolson; Cobo, Justo; Nogueras, Manuel; Sanchez, Adolfo; Quiroga, Jairo; Mejia, Diana

CORPORATE SOURCE: Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen, AB24 3UE, UK

SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (2001), C57(11), 1356-1358

CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mols. of the title compound, C<sub>28</sub>H<sub>27</sub>ClN<sub>4</sub>O<sub>4</sub>·C<sub>2</sub>H<sub>6</sub>O, form a C(6) chain via an N-H...O H bond along the c axis by the operation of a c-glide plane, with N...O = 2.761(3) Å and N-H...O = 165°. The mols. are further linked by a weak C-H...O interaction, with C...O = 3.344(4) Å and C-H...O = 150°. Pendant H-bonded EtOH solvent mols. are attached to the chains by O-H...N H bonds, with O...N = 2.904(3) Å and O-H...N = 175°. Crystallog. data are given.

IT 382591-38-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 382591-38-0 HCAPLUS

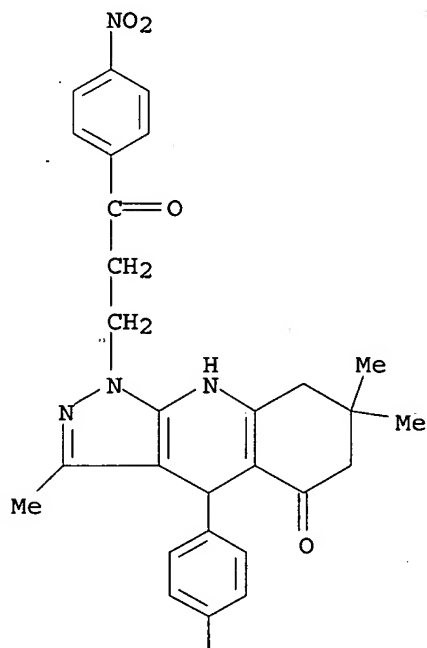
CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-(4-chlorophenyl)-1,4,6,7,8,9-hexahydro-3,7,7-trimethyl-1-[3-(4-nitrophenyl)-3-oxopropyl]-, compd. with ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 382591-37-9

CMF C28 H27 Cl N4 O4

PAGE 1-A



PAGE 2-A

Cl

CM 2

CRN 64-17-5

CMF C2 H6 O

 $\text{H}_3\text{C}-\text{CH}_2-\text{OH}$ 

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:538846 HCAPLUS

DOCUMENT NUMBER: 135:331371

TITLE: Regioselective synthesis of 4,7,8,9-tetrahydro-2H-pyrazolo[3,4-b]quinolin-5(6H)-ones. Mechanism and structural analysis

AUTHOR(S): Quiroga, J.; Mejia, D.; Insuasty, B.; Abonia, R.; Nogueras, M.; Sanchez, A.; Cobo, J.; Low, J. N.

CORPORATE SOURCE: Departamento de Quimica, Grupo de Investigacion de Compuestos Heterociclicos, Universidad del Valle, Cali, 25360, Colombia

SOURCE: Tetrahedron (2001), 57(32), 6947-6953

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:331371

AB Reactions of 5-amino-3-methyl-1H-pyrazole with dimedone and aldehydes afford regioselectively tricyclic linear 3,7,7-trimethyl-4,7,8,9-tetrahydro-2H-pyrazolo[3,4-b]quinolin-5(6H)-ones I (R = Ph, 3-pyridinyl,  $\beta$ -naphthalenyl, etc.) in good yields. Several aspects on this regioselective reaction, such as the reaction mechanism and structural studies of the predominant tautomeric form, are investigated.

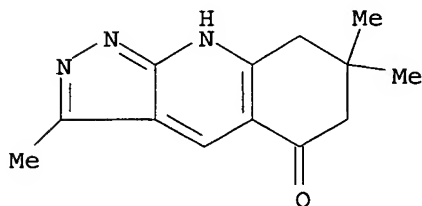
IT 370588-30-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective synthesis of pyrazoloquinolinones by cyclocondensation of aldehydes with aminomethylpyrazole and dimedone and mechanism)

RN 370588-30-0 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 1,6,7,8-tetrahydro-3,7,7-trimethyl-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

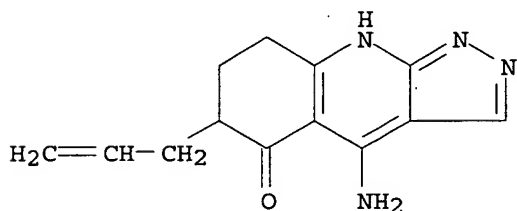
ACCESSION NUMBER: 1996:117818 HCAPLUS  
 DOCUMENT NUMBER: 124:260921  
 TITLE: Trimethylaluminum-promoted cyclization of cyanoenaminones. A versatile synthesis of substituted pyrazolopyridines  
 AUTHOR(S): Campbell, James B.; Firor, Judy W.  
 CORPORATE SOURCE: Medicinal Chem. Dep., Zeneca Pharmaceuticals, Wilmington, DE, 19897, USA  
 SOURCE: Synthetic Communications (1996), 26(5), 981-90  
 CODEN: SYNCAV; ISSN: 0039-7911  
 PUBLISHER: Dekker  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 124:260921

AB The readily available and inexpensive trimethylaluminum was used to effect the facile cyclization of cyanoenaminones to give the corresponding pyrazolopyridine derivs. Certain functional groups and sensitive side-chains, such as the 2-chloroethyl group, nitrile and alkyne, may be accommodated by the reaction.

IT 99162-92-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyrazolopyridines by trimethylaluminum-promoted cyclization of cyanoenaminones)

RN 99162-92-2 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-amino-1,6,7,8-tetrahydro-6-(2-propenyl)- (9CI) (CA INDEX NAME)

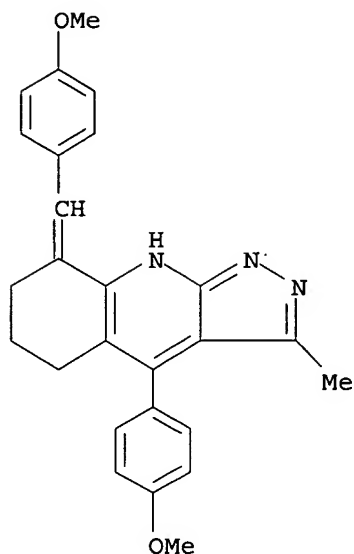


L36 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

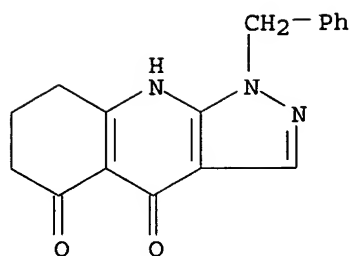
ACCESSION NUMBER: 1994:605193 HCAPLUS  
 DOCUMENT NUMBER: 121:205193  
 TITLE: Reactions with 4-p-anisyl -8-p-anisylidene-1,2,5,6,7,8-hexahydro-2-oxo-3-quinolinecarbonitrile  
 AUTHOR(S): El-Nagdy, S.; Hamad, M.M.; Mahmoud, M.R.; Said, S.A.; Habashy, M.M.  
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
 SOURCE: Egyptian Journal of Chemistry (1992), Volume Date 1991, 34(2), 157-64  
 CODEN: EGJCA3; ISSN: 0367-0422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 121:205193

AB Reactions of the title compound (I) with Et bromoacetate, MeMgI, and POCl3 were studied. Thus, treatment of I with POCl3 gave II which reacted with hydrazine, phenylhydrazine, aniline, benzyl amine, p-toluidine, cyanoacetamide and 2-phenylethanoic hydrazide, in absolute ethanol to yield III (R=NH2, PhNH, Ph, PhCH2, p-MeC6H4, COCH2CN, PhCH2CONH).

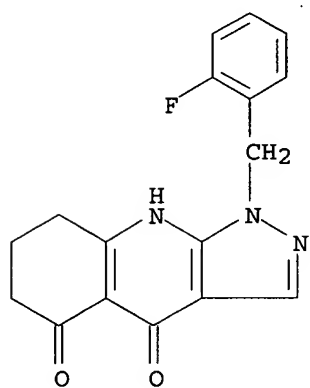
IT 157924-10-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 157924-10-2 HCAPLUS  
 CN 1H-Pyrazolo[3,4-b]quinoline, 5,6,7,8-tetrahydro-4-(4-methoxyphenyl)-8-[(4-methoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)



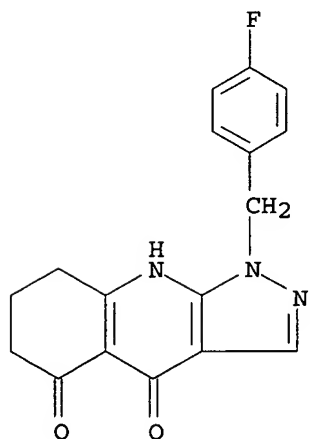
L36 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1991:656057 HCAPLUS  
 DOCUMENT NUMBER: 115:256057  
 TITLE: Synthesis of 7,8-dihydro-6H-pyrazolo[3,4-b]quinolin-5-ones and related derivatives  
 AUTHOR(S): Gatta, Franco; Pomponi, Massimo; Marta, Maurizio  
 CORPORATE SOURCE: Lab. Chim. Farm., Ist. Super. Sanita, Rome, 00161, Italy  
 SOURCE: Journal of Heterocyclic Chemistry (1991), 28(5), 1301-7  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The synthesis of a new series of 4-amino-1-(unsubstituted and chloro or fluoro substituted benzyl)dihydropyrazoloquinolinones I (R = CH<sub>2</sub>Ph, 2-, 4-FC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub> or 2,4-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>) and the corresponding diones II. from the corresponding benzylaminopyrazoles III (R<sub>1</sub> = CN, CO<sub>2</sub>H, CO<sub>2</sub>Et) is reported. The cyclocondensation of I or II with NaN<sub>3</sub> gave azepinones IV or isoxazoles V, resp.  
 IT 137279-14-2P 137279-15-3P 137279-16-4P  
 137279-17-5P 137279-18-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation of, with sodium nitride)  
 RN 137279-14-2 HCAPLUS  
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 7,8-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



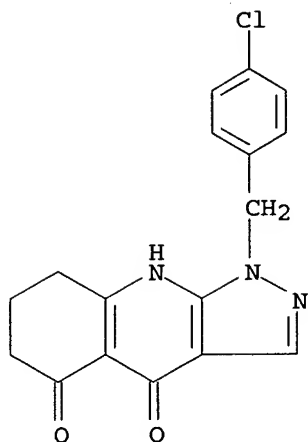
RN 137279-15-3 HCAPLUS  
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(2-fluorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



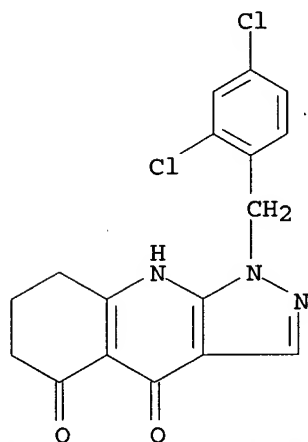
RN 137279-16-4 HCAPLUS  
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(4-fluorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



RN 137279-17-5 HCAPLUS  
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(4-chlorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



RN 137279-18-6 HCAPLUS  
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(2,4-dichlorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



L36 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1986:608800 HCAPLUS  
 DOCUMENT NUMBER: 105:208800  
 TITLE: Phosphorus pentoxide in organic synthesis. XXIX. Synthesis of 4-arylamino-5,6,7,8-tetrahydro-1H-pyrazolo[3,4-b]quinolines and the corresponding N-Mannich bases  
 AUTHOR(S): Nielsen, Soren V.; Pedersen, Erik B.  
 CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.  
 SOURCE: Liebigs Annalen der Chemie (1986), (10), 1728-35  
 CODEN: LACHDL; ISSN: 0170-2041  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:208800  
 AB Title pyrazoloquinolines I (R = H, R1 = arylamino) (II) were prepared (8-52%

IT 103259-41-2P

RN 103259-41-2 HCAPLUS

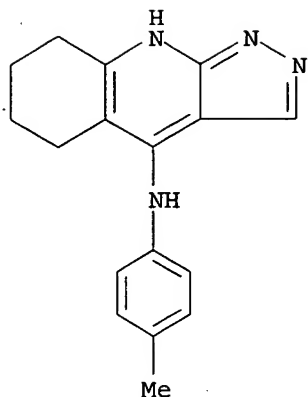
C1=CC=C(C=C1)NC2=C(C3=CC=CC=C3)C(=N4C=CC=CC4)C5=CC=CC=C25

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation, aminomethylation, and spectra of)

RN 103259-36-5 HCAPLUS

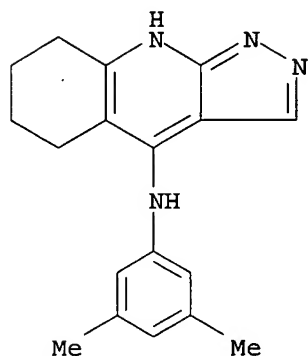
RN 103259-37-6 HCAPLUS

Searched by Paul Schulwitz



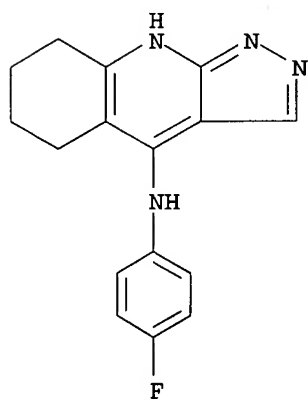
RN 103259-38-7 HCAPLUS

CN 1H-Pyrazolo[3,4-b]quinolin-4-amine, N-(3,5-dimethylphenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 103259-39-8 HCAPLUS

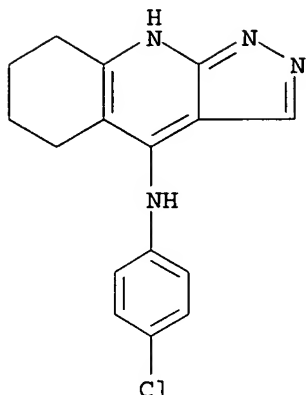
CN 1H-Pyrazolo[3,4-b]quinolin-4-amine, N-(4-fluorophenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 103259-40-1 HCAPLUS

CN 1H-Pyrazolo[3,4-b]quinolin-4-amine, N-(4-chlorophenyl)-5,6,7,8-tetrahydro-

(9CI) (CA INDEX NAME)



L36 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:615280 HCAPLUS

DOCUMENT NUMBER: 103:215280

TITLE: Pyrazolopyridine cycloalkanone derivatives

INVENTOR(S): Campbell, James Boniface, Jr.; Bare, Thomas Michael

PATENT ASSIGNEE(S): ICI Americas, Inc., USA

SOURCE: Eur. Pat. Appl., 115 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.                                    | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| EP 141608                                     | A2   | 19850515 | EP 1984-307272  | 19841023 |
| EP 141608                                     | A3   | 19880302 |                 |          |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE |      |          |                 |          |
| US 4546104                                    | A    | 19851008 | US 1984-659615  | 19841011 |
| ZA 8408352                                    | A    | 19850626 | ZA 1984-8352    | 19841025 |
| FI 8404296                                    | A    | 19850505 | FI 1984-4296    | 19841101 |
| DK 8405229                                    | A    | 19850505 | DK 1984-5229    | 19841102 |
| NO 8404376                                    | A    | 19850506 | NO 1984-4376    | 19841102 |
| AU 8434949                                    | A1   | 19850509 | AU 1984-34949   | 19841102 |
| HU 35679                                      | O    | 19850729 | HU 1984-4064    | 19841102 |
| ES 537338                                     | A1   | 19860101 | ES 1984-537338  | 19841102 |
| JP 60115581                                   | A2   | 19850622 | JP 1984-231445  | 19841105 |

PRIORITY APPLN. INFO.: GB 1983-29531 19831104

AB The title compds. [I: R, R2 = H, (substituted) alkyl; R1 = H, alkyl; R3, R4 = H, (substituted) alkyl, CR3R4 = ring; R5, R6 = H, alkyl, alkenyl; X = bond, alkylene] were prepared. Thus, heating a mixture 1.65 g pyrazole derivative

II, 20 mL xylenes, and 12 g ZnCl<sub>2</sub> for 2 h gave 0.68 g I (R = pentyl, R1-R6 = H, X = CH<sub>2</sub>). All I exhibited anxiolytic activity in rats.

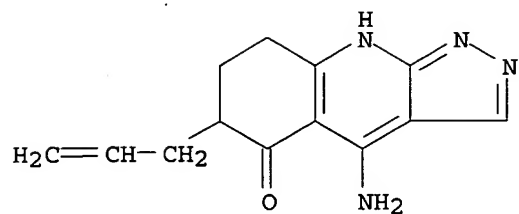
IT 99162-92-2P 99162-95-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and alkylation and anxiolytic activity of)

RN 99162-92-2 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-amino-1,6,7,8-tetrahydro-6-(2-

propenyl)- (9CI) (CA INDEX NAME)



RN 99162-95-5 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-amino-6-(3,3-dichloro-2-propenyl)-  
1,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

